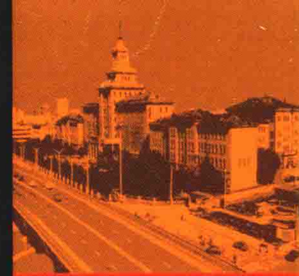
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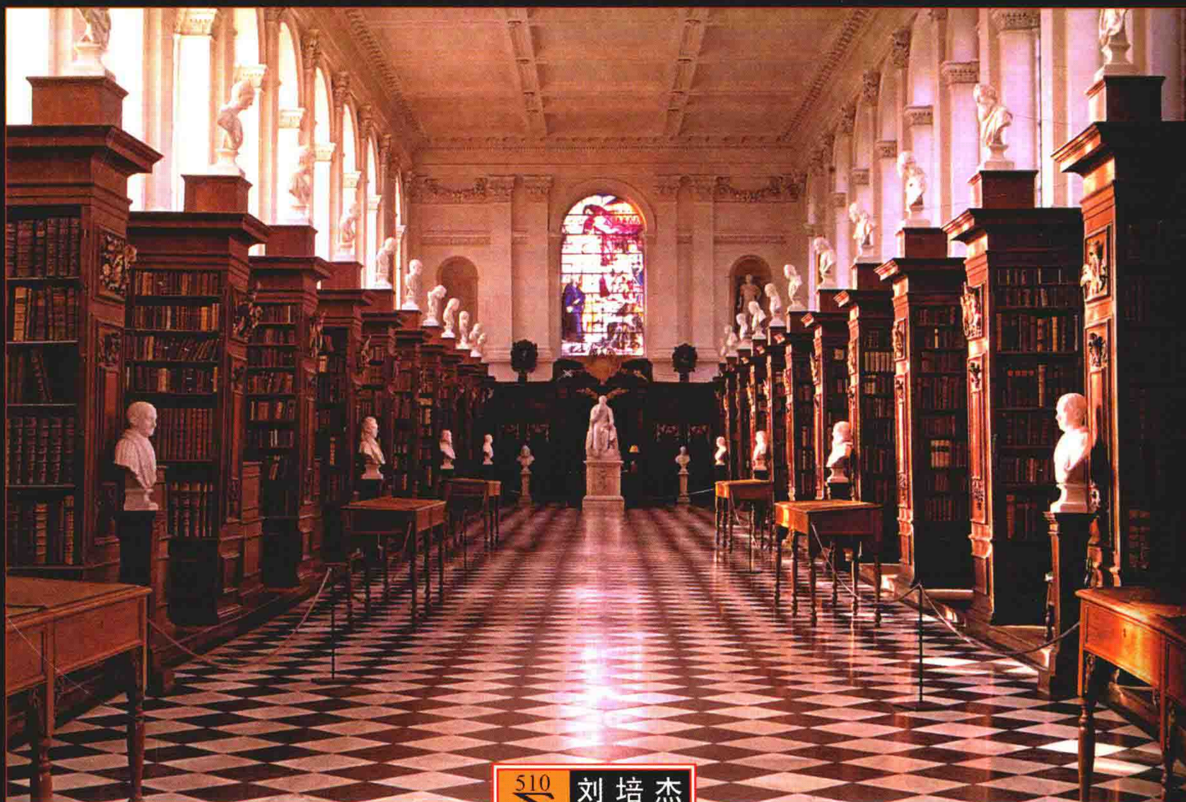
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（第3卷）

Francoise, J.P.（弗朗索瓦斯） Naber, G.L.（纳伯） Tsou Sheung Tsun（孙圣周） 著

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FOREWORD

In bygone centuries, our physical world appeared to be filled to the brim with mysteries. Divine powers could provide for genuine miracles; water and sunlight could turn arid land into fertile pastures, but the same powers could lead to miseries and disasters. The force of life, the *vis vitalis*, was assumed to be the special agent responsible for all living things. The heavens, whatever they were for, contained stars and other heavenly bodies that were the exclusive domain of the Gods.

Mathematics did exist, of course. Indeed, there was one aspect of our physical world that was recognised to be controlled by precise, mathematical logic: the geometric structure of space, elaborated to become a genuine form of art by the ancient Greeks. From my perspective, the Greeks were the first practitioners of 'mathematical physics', when they discovered that all geometric features of space could be reduced to a small number of axioms. Today, these would be called 'fundamental laws of physics'. The fact that the flow of *time* could be addressed with similar exactitude, and that it could be handled geometrically together with space, was only recognised much later. And, yes, there were a few crazy people who were interested in the magic of numbers, but the real world around us seemed to contain so much more that was way beyond our capacities of analysis.

Gradually, all this changed. The Moon and the planets appeared to follow geometrical laws. Galilei and Newton managed to identify their logical rules of motion, and by noting that the concept of mass could be applied to things in the sky just like apples and cannon balls on Earth, they made the sky a little bit more accessible to us. Electricity, magnetism, light and sound were also found to behave in complete accordance with mathematical equations.

Yet all of this was just a beginning. The real changes came with the twentieth century. A completely new way of thinking, by emphasizing mathematical, logical analysis rather than empirical evidence, was pioneered by Albert Einstein. Applying advanced mathematical concepts, only known to a few pure mathematicians, to notions as mundane as space and time, was new to the physicists of his time. Einstein himself had a hard time struggling through the logic of connections and curvatures, notions that were totally new to him, but are only too familiar to students of mathematical physics today. Indeed, there is no better testimony of Einstein's deep insights at that time, than the fact that we now teach these things regularly in our university classrooms.

Special and general relativity are only small corners of the realm of modern physics that is presently being studied using advanced mathematical methods. We have notoriously complex subjects such as phase transitions in condensed matter physics, superconductivity, Bose–Einstein condensation, the quantum Hall effect, particularly the fractional quantum Hall effect, and numerous topics from elementary particle physics, ranging from fibre bundles and renormalization groups to supergravity, algebraic topology, superstring theory, Calabi–Yau spaces and what not, all of which require the utmost of our mental skills to comprehend them.

The most bewildering observation that we make today is that it seems that our *entire* physical world appears to be controlled by mathematical equations, and these are not just sloppy and debatable models, but precisely documented properties of materials, of systems, and of phenomena in all echelons of our universe.

Does this really apply to our entire world, or only to parts of it? Do features, notions, entities exist that are emphatically *not* mathematical? What about intuition, or dreams, and what about consciousness? What about religion? Here, most of us would say, one should not even try to apply mathematical analysis, although even here, some brave social scientists are making attempts at coordinating rational approaches.

No, there are clear and important differences between the physical world and the mathematical world. Where the physical world stands out is the fact that it refers to 'reality', whatever 'reality' is. Mathematics is the world of pure logic and pure reasoning. In physics, it is the experimental evidence that ultimately decides whether a theory is acceptable or not. Also, the methodology in physics is different.

A beautiful example is the serendipitous discovery of superconductivity. In 1911, the Dutch physicist Heike Kamerlingh Onnes was the first to achieve the liquefaction of helium, for which a temperature below 4.25 K had to be realized. Heike decided to measure the specific conductivity of mercury, a metal that is frozen solid at such low temperatures. But something appeared to go wrong during the measurements, since the volt meter did not show any voltage at all. All experienced physicists in the team assumed that they were dealing with a malfunction. It would not have been the first time for a short circuit to occur in the electrical equipment, but, this time, in spite of several efforts, they failed to locate it. One of the assistants was responsible for keeping the temperature of the sample well within that of liquid helium, a dull job, requiring nothing else than continuously watching some dials. During one of the many tests, however, he dozed off. The temperature rose, and suddenly the measurements showed the normal values again. It then occurred to the investigators that the effect and its temperature dependence were completely reproducible. Below 4.19 degrees Kelvin the conductivity of mercury appeared to be strictly infinite. Above that temperature, it is finite, and the transition is a very sudden one. Superconductivity was discovered (D. van Delft, "Heike Kamerling Onnes", Uitgeverij Bert Bakker, Amsterdam, 2005 (in Dutch)).

This is not the way mathematical discoveries are made. Theorems are not produced by assistants falling asleep, even if examples do exist of incidents involving some miraculous fortune.

The hybrid science of mathematical physics is a very curious one. Some of the topics in this Encyclopedia are undoubtedly physical. High T_c superconductivity, breaking water waves, and magneto-hydrodynamics, are definitely topics of physics where experimental data are considered more decisive than any high-brow theory. Cohomology theory, Donaldson–Witten theory, and AdS/CFT correspondence, however, are examples of purely mathematical exercises, even if these subjects, like all of the others in this compilation, are strongly inspired by, and related to, questions posed in physics.

It is inevitable, in a compilation of a large number of short articles with many different authors, to see quite a bit of variation in style and level. In this Encyclopedia, theoretical physicists as well as mathematicians together made a huge effort to present in a concise and understandable manner their vision on numerous important issues in advanced mathematical physics. All include references for further reading. We hope and expect that these efforts will serve a good purpose.

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PREFACE

Mathematical Physics as a distinct discipline is relatively new. The International Association of Mathematical Physics was founded only in 1976. The interaction between physics and mathematics has, of course, existed since ancient times, but the recent decades, perhaps partly because we are living through them, appear to have witnessed tremendous progress, yielding new results and insights at a dizzying pace, so much so that an encyclopedia seems now needed to collate the gathered knowledge.

Mathematical Physics brings together the two great disciplines of Mathematics and Physics to the benefit of both, the relationship between them being symbiotic. On the one hand, it uses mathematics as a tool to organize physical ideas of increasing precision and complexity, and on the other it draws on the questions that physicists pose as a source of inspiration to mathematicians. A classical example of this relationship exists in Einstein's theory of relativity, where differential geometry played an essential role in the formulation of the physical theory while the problems raised by the ensuing physics have in turn boosted the development of differential geometry. It is indeed a happy coincidence that we are writing now a preface to an encyclopedia of mathematical physics in the centenary of Einstein's annus mirabilis.

The project of putting together an encyclopedia of mathematical physics looked, and still looks, to us a formidable enterprise. We would never have had the courage to undertake such a task if we did not believe, first, that it is worthwhile and of benefit to the community, and second, that we would get the much-needed support from our colleagues. And this support we did get, in the form of advice, encouragement, and practical help too, from members of our Editorial Advisory Board, from our authors, and from others as well, who have given unstintingly so much of their time to help us shape this Encyclopedia.

Mathematical Physics being a relatively new subject, it is not yet clearly delineated and could mean different things to different people. In our choice of topics, we were guided in part by the programs of recent International Congresses on Mathematical Physics, but mainly by the advice from our Editorial Advisory Board and from our authors. The limitations of space and time, as well as our own limitations, necessitated the omission of certain topics, but we have tried to include all that we believe to be core subjects and to cover as much as possible the most active areas.

Our subject being interdisciplinary, we think it appropriate that the Encyclopedia should have certain special features. Applications of the same mathematical theory, for instance, to different problems in physics will have different emphasis and treatment. By the same token, the same problem in physics can draw upon resources from different mathematical fields. This is why we divide the Encyclopedia into two broad sections: physics subjects and related mathematical subjects. Articles in either section are deliberately allowed a fair amount of overlap with one another and many articles will appear under more than one heading, but all are linked together by elaborate cross referencing. We think this gives a better picture of the subject as a whole and will serve better a community of researchers from widely scattered yet related fields.

The Encyclopedia is intended primarily for experienced researchers but should be of use also to beginning graduate students. For the latter category of readers, we have included eight elementary introductory articles for easy reference, with those on mathematics aimed at physics graduates and those on physics aimed at mathematics graduates, so that these articles can serve as their first port of call to enable them to embark on any of the main articles without the need to consult other material beforehand. In fact, we think these articles may even form the

foundation of advanced undergraduate courses, as we know that some authors have already made such use of them.

In addition to the printed version, an on-line version of the Encyclopedia is planned, which will allow both the contents and the articles themselves to be updated if and when the occasion arises. This is probably a necessary provision in such a rapidly advancing field.

This project was some four years in the making. Our foremost thanks at its completion go to the members of our Editorial Advisory Board, who have advised, helped and encouraged us all along, and to all our authors who have so generously devoted so much of their time to writing these articles and given us much useful advice as well. We ourselves have learnt a lot from these colleagues, and made some wonderful contacts with some among them. Special thanks are due also to Arthur Greenspoon whose technical expertise was indispensable.

The project was started with Academic Press, which was later taken over by Elsevier. We thank warmly members of their staff who have made this transition admirably seamless and gone on to assist us greatly in our task: both Carey Chapman and Anne Guillaume, who were in charge of the whole project and have been with us since the beginning, and Edward Taylor responsible for the copy-editing. And Martin Ruck, who manages to keep an overwhelming amount of details constantly at his fingertips, and who is never known to have lost a single email, deserves a very special mention.

As a postscript, we would like to express our gratitude to the very large number of authors who generously agreed to donate their honorariums to support the Committee for Developing Countries of the European Mathematical Society in their work to help our less fortunate colleagues in the developing world.

Jean-Pierre Françoise
Gregory L. Naber
Tsou Sheung Tsun

GUIDE TO USE OF THE ENCYCLOPEDIA

Structure of the Encyclopedia

The material in this Encyclopedia is organised into two sections. At the start of Volume 1 are eight **Introductory Articles.** The introductory articles on mathematics are aimed at physics graduates; those on physics are aimed at mathematics graduates. It is intended that these articles should serve as the first port of call for graduate students, to enable them to embark on any of the main entries without the need to consult other material beforehand.

Following the Introductory Articles, the main body of the Encyclopedia is arranged as a series of entries in alphabetical order. These entries fill the remainder of Volume 1 and all of the subsequent volumes (2–5).

To help you realize the full potential of the material in the Encyclopedia we have provided four features to help you find the topic of your choice: a contents list by subject, an alphabetical contents list, cross-references, and a full subject index.

1. Contents List by Subject

Your first point of reference will probably be the contents list by subject. This list appears at the front of each volume, and groups the entries under subject headings describing the broad themes of mathematical physics. This will enable the reader to make quick connections between entries and to locate the entry of interest. The contents list by subject is divided into two main sections: *Physics Subjects* and *Related Mathematics Subjects*. Under each main section heading, you will find several subject areas (such as GENERAL RELATIVITY in Physics Subjects or NONCOMMUTATIVE GEOMETRY in Related Mathematics Subjects). Under each subject area is a list of those entries that cover aspects of that subject, together with the volume and page numbers on which these entries may be found.

Because mathematical physics is so highly interconnected, individual entries may appear under more than one subject area. For example, the entry GAUGE THEORY: MATHEMATICAL APPLICATIONS is listed under the Physics Subject GAUGE THEORY as well as in a broad range of Related Mathematics Subjects.

2. Alphabetical Contents List

The alphabetical contents list, which also appears at the front of each volume, lists the entries in the order in which they appear in the Encyclopedia. This list provides both the volume number and the page number of the entry.

You will find "dummy entries" where obvious synonyms exist for entries or where we have grouped together related topics. Dummy entries appear in both the contents list and the body of the text.

Example

If you were attempting to locate material on path integral methods via the alphabetical contents list:

PATH INTEGRAL METHODS *see* Functional Integration in Quantum Physics; Feynman Path Integrals

The dummy entry directs you to two other entries in which path integral methods are covered. At the appropriate locations in the contents list, the volume and page numbers for these entries are given.

If you were trying to locate the material by browsing through the text and you had looked up Path Integral Methods, then the following information would be provided in the dummy entry:

Path Integral Methods *see* Functional Integration in Quantum Physics; Feynman Path Integrals

3. Cross-References

All of the articles in the Encyclopedia have been extensively cross-referenced. The cross-references, which appear at the end of an entry, serve three different functions:

i. To indicate if a topic is discussed in greater detail elsewhere.

ii. To draw the reader's attention to parallel discussions in other entries.

iii. To indicate material that broadens the discussion.

Example
The following list of cross-references appears at the end of the entry STOCHASTIC HYDRODYNAMICS

> *See also*: Cauchy Problem for Burgers-Type Equations; Hamiltonian Fluid Dynamics; Incompressible Euler Equations: Mathematical Theory; Malliavin Calculus; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Stochastic Differential Equations; Turbulence Theories; Viscous Incompressible Fluids: Mathematical Theory; Vortex Dynamics

Here you will find examples of all three functions of the cross-reference list: a topic discussed in greater detail elsewhere (e.g. Incompressible Euler Equations: Mathematical Theory), parallel discussion in other entries (e.g. Stochastic Differential Equations) and reference to entries that broaden the discussion (e.g. Turbulence Theories).

The eight Introductory Articles are not cross-referenced from any of the main entries, as it is expected that introductory articles will be of general interest. As mentioned above, the Introductory Articles may be found at the start of Volume 1.

4. Index

The index will provide you with the volume and page number where the material is located. The index entries differentiate between material that is a whole entry, is part of an entry, or is data presented in a figure or table. Detailed notes are provided on the opening page of the index.

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Image Processing: Mathematics

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Our society is often designated as being an "information society." It could also be defined as an "image society." This is not only because image is a powerful and widely used medium of communication, but also because it is an easy, compact, and widespread way to represent the physical world. If we think about it, it is indeed striking to realize just how much images are omnipresent in our lives through numerous applications such as medical and satellite imaging, videosurveillance, cinema, robotics, etc.

Many approaches have been developed to process these digital images, and it is difficult to say which one is more natural than the other. Image processing has a long history. Maybe the oldest methods come from 1D signal processing techniques. They rely on filter theory (linear or not), on spectral analysis, or on some basic concepts of probability and statistics. For an overview, we refer the interested reader to the book by Gonzalez and Woods (1992).

In this article, some recent mathematical concepts will be revisited and illustrated by the image restoration problem, which is presented below. We first discuss stochastic modeling which is widely based on Markov random field theory and deals directly with digital images. This is followed by a discussion of variational approaches where the general idea is to define some cost functions in a continuous setting. Next we show how the scale space theory is connected with partial differential equations (PDEs). Finally, we present the wavelet theory, which is inherited from signal processing and relies on decomposition techniques.

Introduction

As in the real world, a digital image is composed of a wide variety of structures. **Figure 1** shows different kinds of "textures," progressive or sharp contours, and fine objects. This gives an idea of the complexity of finding an approach that allows to cope with the different structures at the same time. It also highlights the discrete nature of images which will be handled differently depending on the chosen mathematical tools. For instance, PDEs based approaches are written in a continuous setting, referring to analogous images, and once the existence and the uniqueness of the solution have been proved, we need to discretize them in order to find a numerical solution. On the contrary, stochastic approaches will directly consider discrete images in the modeling of the cost functions.

The Image Restoration Problem

It is well known that during formation, transmission, and recording processes images deteriorate. Classically, this degradation is the result of two phenomena. The first one is deterministic and is related to the image acquisition modality, to possible defects of the imaging system (e.g., blur created by an incorrect lens adjustment or by motion). The second phenomenon is random and corresponds to the noise coming from any signal transmission. It can also come from image quantization. It is important to choose a degradation model as close as possible to reality. The random noise is usually modeled by a probabilistic distribution. In many cases, a Gaussian distribution is assumed. However, some applications require more specific ones, like the gamma distribution for radar images (speckle noise) or the Poisson distribution for tomography. Unfortunately, it is usually impossible to identify the kind of noise involved for a given real image.

A commonly used model is the following. Let $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$ be an original image describing a real scene, and let f be the observed image of the same scene (i.e., a degradation of u). We assume that

$$f = Au + \eta \qquad [1]$$

where η stands for a white additive Gaussian noise and A is a linear operator representing the blur (usually a convolution). Given f, the problem is

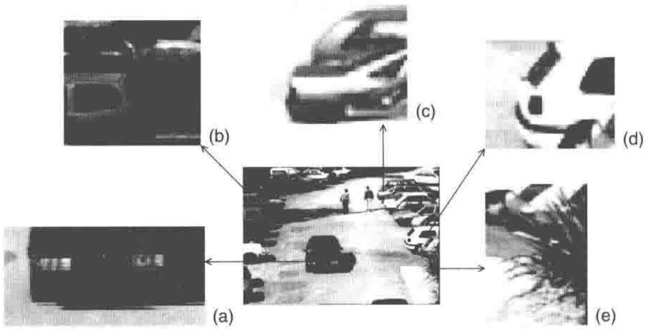


Figure 1 Digital image example. ↷ the close-ups show examples of low resolution, low contrasts, graduated shadings, sharp transitions, and fine elements. (a) low resolution, (b) low contrasts, (c) graduated shadings, (d) sharp transitions, and (e) fine elements.

then to reconstruct u knowing [1]. This problem is ill-posed, and we are able to carry out only an approximation of u. In this article, we will focus on the simplified model of pure denoising:

$$f = u + \eta \qquad [2]$$

The Probabilistic Approach

The Bayesian Framework

In this section, we show how the problem of pure denoising, that is, recovering u from the equation $f = u + \eta$ knowing only some statistical information on η can be solved by using a probabilistic approach. In this context, f, u, and η are considered as random variables. The general idea for recovering u is to maximize some prior probability. Most models involve two parts: a prior model of possible restored images u and a data model expressing consistency with the observed data.

- The prior model is given by a probability space (Ω_u, p), where Ω_u is the set of all values of u. The model is specified by giving the probability $p(u)$ on all these values.
- The data model is a larger probability space $(\Omega_{u,f}, p)$, where $\Omega_{u,f}$ is the set of all possible values of u and all possible values of the observed image f. This model is completed by giving the conditional probability $p(f/u)$ of any image f given u, resulting in the joint probabilities $p(f,u) = p(f/u)p(u)$. Implicitly, we assume that the spaces (Ω_u) and $(\Omega_{u,f})$ are finite although huge.

The next step is to use a Bayesian approach introduced in image processing by Besag (1974) and Geman and Geman (1984). The probabilities $p(u)$ and $p(f/u)$ are supposed to be known and, given an observed image f, we seek the image u which maximizes the conditional *a posteriori* probability $p(u/f)$ (MAP: Maximum A Posteriori). Thanks to the Bayes' rule, we have

$$p(u/f) = \frac{p(f/u)p(u)}{p(f)} \qquad [3]$$

Let us explain the meaning of the different terms in [3]:

- The term $p(f/u)$ expresses the probability, the likelihood, that an image u is realized in f. It also quantifies the lack of total precision of the model and the presence of noise.
- The term $p(u)$ expresses our incomplete *a priori* information about the ideal image u (it is the probability of the model, i.e., the propensity that u be realized independently of the observation f).
- The term $p(f)$ which is the probability to observe f is a constant and does not play any role when maximizing the conditional probability $p(u/f)$ with respect to u.

Let us remark that the problem $\max_u p(u/f)$ is equivalent to $\min_u E(u) = -\log p(f/u) - \log p(u)$. So Bayesian models lead to a minimization process.

Then the main question is how to assign these probabilities? The easiest probability to determine is $p(f/u)$. If the images u and f consist in a set of values $u = (u_{i,j}), i,j = 1,N$ and $f = (f_{i,j}), i,j = 1,N$, we suppose the conditional independence of $(f_{i,j}/u_{i,j})$ in any pixel:

$$p(f/u) = \prod_{i=1}^{N} p(f_{i,j}/u_{i,j})$$

and if the restoration model is of the form $f = u + \eta$ where η is a white Gaussian noise with variance σ^2, then

$$p(f_{i,j}/u_{i,j}) = \frac{1}{\sqrt{2\pi}\sigma} \exp - \frac{(f_{i,j} - u_{i,j})^2}{2\sigma^2}$$

and

$$p(f/u) = \frac{1}{(2\pi\sigma)^{N/2}} \exp - \sum_{i,j}^{N} \frac{(f_{i,j} - u_{i,j})^2}{2\sigma^2}$$

Therefore, at this stage, the MAP reduces to minimize

$$E(u) = K_\sigma \|f - u\|^2 - \log p(u) \qquad [4]$$

where $\|.\|$ stands for the Euclidean norm on $\mathbb{R}^{N^2}$ and K_σ is a constant. So, it remains now to assign a probability law $p(u)$. To do that, the most common way is to use the theory of Markov random fields (MRFs).

The Theory of Markov Random Fields

In this approach, an image is described as a finite set S of sites corresponding to the pixels. For each site, we associate a descriptor representing the state of the site, for example, its gray level. In order to take into account local interaction between sites, one needs to endow S with a system of neighborhoods $\mathcal{V}$.

Definition 1 For each site s, we define its neighborhood $\mathcal{V}(s)$ as:

$$\mathcal{V}(s) = \{t\} \text{ such that } s \notin \mathcal{V}(s) \text{ and } t \in \mathcal{V}(s) \Rightarrow s \in \mathcal{V}(t)$$

Then we associate to this neighborhood system the notion of clique: a clique is either a singleton or a set of sites which are all neighbors of each other. Depending on the neighborhood system, the family of cliques will be different and involve more and less sites. We will denote by $\mathcal{C}$ the set of all the cliques relative to a neighborhood system $\mathcal{V}$ (see **Figure 2**).

Before introducing the general framework of MRFs, let us define some notations. For a site s, X_s will stand for a random variable taking its values in some set $\mathcal{E}$ (e.g., $\mathcal{E} = \{0, 1, \ldots, 255\}$) and x_s will be a realization of X_s and $x^s = (x_t)_{t \neq s}$ will denote an image configuration where site s has been removed. Finally, we will denote by X the random variable $X = (X_s, X_t, \ldots)$ with values in $\Omega = \mathcal{E}^{|S|}$.

Definition 2 We say that X is an MRF if the local conditional probability at a site s is only a function of $\mathcal{V}(s)$, that is,

$$p(X_s = x_s / X^s = x^s) = p(X_s = x_s / x_t, t \in \mathcal{V}(s))$$

Therefore, the gray level at a site depends only on gray levels of neighboring pixels. Now we give the following fundamental theorem due to Hammersley–Clifford (Besag 1974) which states the equivalence between MRFs and Gibbs fields.

Theorem 1 *Let us suppose that S is finite, $\mathcal{E}$ is a discrete set and for all $x \in \Omega = \mathcal{E}^{|S|}, p(X = x) > 0$, then X is an MRF relatively to a system of neighborhoods $\mathcal{V}$ if and only if there exists a family of potential functions $(V_c)_{c \in \mathcal{C}}$ such that $p(x) = (1/Z)\exp(-\sum_{c \in \mathcal{C}} V_c(x))$.*

The function $V(x) = \sum_{c \in \mathcal{C}} V_c(x)$ is called the energy potential or the Gibbs measure and Z is a normalizing constant: $Z = \exp(-\sum_{x \in \Omega} V(x))$.

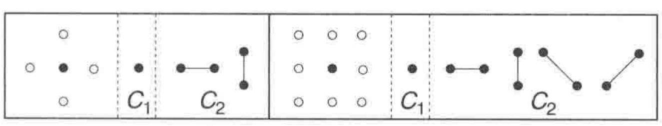


Figure 2 Examples of neighborhood system and cliques.

If, for example, the collection of neighborhoods is the set of 4-neighbors, then the theorem says that $V(x) = \sum_{c = \{s\} \in C_1} V_c(x_s) + \sum_{c = \{(s,t)\} \in C_2} V_c(x_s, x_t)$.

Application to the Denoising Problem

Now, given this theorem we can reformulate, thanks to [4], the restoration problem (with the change of notation $u = x$ and $u_s = x_s$): find u minimizing the global energy

$$E(u) = K_\sigma \|f - u\|^2 + V(u) \qquad [5]$$

The next step is now to precise the Gibbs measure. In restoration, the potential $V(u)$ is often dedicated to impose local regularity constraints, for example, by penalizing differences between neighbors. This can be modeled using cliques of order 2 in the following manner:

$$V(u) = \beta \sum_{(s,t) \in \mathcal{C}_2} \phi(u_s - u_t)$$

where ϕ is a given real function. This term penalizes the difference of intensities between neighbors which may come from an edge or some noise. This discrete cost function is very similar to the gradient penalty terms in the continuous framework (see the next section). The resulting final energy is (sometimes $E(u)$ is written $E(u/f)$)

$$E(u) = K_\sigma \sum_{s \in S} (f_s - u_s)^2 + \beta \sum_{(s,t) \in \mathcal{C}_2} \phi(u_s - u_t)$$

where the constant β is a weighting parameter which can be estimated.

The difficulty in choosing the strength of the penalty term defined by ϕ is to be able to penalize the noise while keeping the most salient features, that is, edges. Historically, the function ϕ was first chosen as $\phi(z) = z^2$ but this choice is not good since the resulting regularization is too strong introducing a blur in the image and loss of the edges. A better choice is $\phi(z) = |z|$ (Rudin *et al.* 1992) or a regularized version of this function. Of course, other choices are possible depending on the considered application and the desired degree of smoothness.

In this section, it has been shown how to model the restoration problem through MRFs and the Bayesian framework. Numerically, two main types of algorithms can be used to minimize the energy: deterministic algorithms and stochastic algorithms. The former are generally used when the global energy is strictly convex (e.g., algorithms based on

gradient descent). The latter are rather used when $E(u)$ is not convex. There are stochastic minimization algorithms mainly based on simulated annealing. Their main interest is that they always converge (almost surely) to a minimizer (this is not the case for deterministic algorithms which give only local minimizers) but they are often strongly time consuming.

We refer the reader to Li (1995) for more details about MRFs and Bayesian framework and Kirkpatrick *et al.* (1983) for more information on stochastic algorithms.

The Variational Approach

Minimizing a Cost Function over a Functional Space

One important issue in the previous section was the definition of $p(u)$ which gives some *a priori* on the solution. In the variational approach, this idea is also present but the way to infer it is in fact to define the more suitable functional space that describes images and their geometrical properties. The choice of a functional space sets a norm which in turn will constrain the solution to a certain smoothness.

We illustrate this idea in this section on the denoising problem [2] which can be seen as a decomposition one. This means that given the observation f, we look for u and η such that $f = u + \eta$, where η incorporates all oscillations, that is, noise, and also texture. Let us define a functional to be minimized which takes into account the data f and possibly some statistical informations about η:

$$\min_{(u,\eta)}\{\phi(|u|_E) \text{ such that } \psi(|\eta|_G) = \sigma \text{ with } f = u + \eta\} \qquad [6]$$

This formulation means that we look, among all decompositions $f = u + \eta$, for the one which minimizes $\phi(|u|_E)$ under the constraint $\psi(|\eta|_G) = \sigma$. Banach spaces E and G, and functions ϕ and ψ will be discussed in the next subsection. Since a minimization problem under constraints can be expressed with an additional term weighted by a Lagrange multiplier, the formulation [6] can be rewritten as:

$$\min_{(u,\eta)}\{\phi(|u|_E) + \lambda\psi(|\eta|_G); f = u + \eta\} \qquad [7]$$

A similar writing consists in replacing η by $f - u$ so that [7] rewrites

$$\min_{u}\{\phi(|u|_E) + \lambda\psi(|f - u|_G)\} \qquad [8]$$

which is the classical formulation in image restoration. From a numerical point of view, the minimization is usually carried out by solving the associated Euler equations but this may be a difficult task. The main concern is the search for E and G and their norm (or seminorm). It is guided by the choice that an image u is composed of various geometric structures (homogeneous regions, edges) while $\eta = f - u$ represents oscillations (noise and textures).

Examples of Functional Spaces

In this section, we revisit some possible choices of functional spaces summarized in **Table 1**.

The first case (a) was inspired by the classical Tikhonov regularization. The functional space $H^1(\Omega)(\Omega \subset \mathbb{R}^2)$ is the space of functions in $L^2(\Omega)$ such that the distributional gradient Du is in $L^2(\Omega)$. Unfortunately, functions in $H^1(\Omega)$ do not admit discontinuities across curves and this is a major problem with respect to image analysis since images are made of smooth patches separated by sharp variations.

Considering the problem reported in (a), Rudin *et al.* (1992) proposed to work on $\mathrm{BV}(\Omega)$, the space of bounded variations (BV) Ambrosio *et al.* (2000) defined by

$$\mathrm{BV}(\Omega) = \left\{u \in L^1(\Omega); \int_\Omega |Du| < \infty\right\}$$
$$\text{with } \int_\Omega |Du| = \sup\left\{\int_\Omega u \operatorname{div}\varphi \, dx; \varphi = (\varphi_1, \varphi_2, \ldots, \varphi_N) \in \mathcal{C}_0^1(\Omega)^N, |\varphi|_{L^\infty(\Omega)} \leq 1\right\} \qquad [9]$$

Table 1 Examples of functional spaces and their norm (see model [8])

Model	*E* and $\lvert u\rvert_E$	$\phi(t)$	*G* and $\lvert u\rvert_G$	$\psi(t)$
(a)	$H^1(\Omega), \lvert u\rvert_E = \left(\int_\Omega \lvert\nabla u\rvert^2 dx\right)^{1/2}$	t^2	$L^2(\Omega)$ with its usual norm	t^2
(b)	$BV(\Omega), \lvert u\rvert_E = \int_\Omega \lvert Du\rvert$	t	$L^2(\Omega)$ with its usual norm	t^2
(c)	$BV(\Omega), \lvert u\rvert_E = \int_\Omega \lvert Du\rvert$	t	$\{b \in L^2(\Omega); b = \operatorname{div}\xi, \lvert\xi\rvert_{L^\infty(\Omega)^2} \leq 1, \xi \cdot N\rvert_{\partial\Omega} = 0\}$	t

It is equivalent to define $BV(\Omega)$ as the space of $L^1(\Omega)$ functions whose distributional gradient Du is a bounded measure and [9] is its total variation. The space $BV(\Omega)$ has some interesting properties:

1. lower semicontinuity of the total variation $\int_\Omega |Du|$ with respect to the $L^1(\Omega)$ topology,
2. if $u \in BV(\Omega)$, we can define, for $\mathcal{H}^1$ almost everywhere $x \in S_u$, the complement of Lebesgue points (i.e., the jump set of u), a normal $n_u(x)$ and two approximate "right" and "left" limits $u^+(x)$ and $u^-(x)$, and
3. Du can be decomposed as a sum of a regular measure, a jump measure, and a Cantor measure:

$$Du = \nabla u \, dx + (u^+ - u^-) n_u \mathcal{H}^1_{/S_u} + C_u$$

where ∇u is the approximate gradient and $\mathcal{H}^1$ the one-dimensional Hausdorff measure.

This ability to describe functions with discontinuities across a hypersurface S_u makes $BV(\Omega)$ very convenient to describe images with edges. In this context, the image restoration problem is well posed and suitable numerical tools can be proposed (Chambolle and Lions 1997).

One criticism of the model (b) in **Table 1** pointed out by Meyer (2001) is that if f is a characteristic function and if f is sufficiently small with respect to a suitable norm, then the model (Rudin *et al.* 1992) gives $u = 0$ and $\eta = f$ contrary to what one should expect ($u = f$ and $\eta = 0$). In fact, the main reason of this phenomenon is that the L^2-norm for the η component is not the right one since very oscillating functions can have large L^2-norm (e.g., $f_n(x) = \cos(nx)$). To better describe such oscillating functions, Meyer (2001) introduced the space of functions which can be expressed as a divergence of L^∞-fields. This work was developed in R^N and this framework was adapted to bounded 2D domains by Aubert and Aujol (2005) (see (c) in **Table 1**). An example of image decomposition is shown in **Figure 3**.

In this section, we have shown how the choice of the functional spaces is closely related to the definition of a variational formulation. The functionals are written in a continuous setting and they can usually be minimized by solving the discretized Euler equations iteratively, until convergence. These PDEs and the differential operators are constrained by the energy definition but it is also possible to work directly on the equations, forgetting the formal link with the energy. Such an approach has also been much developed in the computer vision community and it is illustrated in the next section.

We refer the reader to Aubert and Kornprobst (2002) for a general review of variational approaches and PDEs as applied to image analysis.



Figure 3 Example of image decomposition (see Aubert and Aujol (2005)).

Scale Spaces and PDEs

Another approach to perform nonlinear filtering is to define a family of image smoothing operators T_t, depending on a scale parameter t. Given an image $f(x)$, we can define the image $u(t,x) = (T_t f)(x)$ which corresponds to the image f analyzed at scale t. In this section, following Alvarez–Guichard–Lions–Morel (Alvarez *et al.* 1993), we show that $u(t,x)$ is the solution of a PDE provided some suitable assumptions on T_t.

Basic Principles of a Scale Space

This section describes some natural assumptions to be fulfilled by scale spaces. We first assume that the output at scale t can be computed from the output at a scale $t - h$ for very small h. This is natural, since a coarser scale view of the original picture is likely to be deduced from a finer one. T_t is obtained by composition of transition filters, denoted by $T_{t+h,t}$. So the first axiom is

(A1) $T_{t+h} = T_{t+h,t} T_t \quad T_0 = \mathrm{Id}$

Another assumption is that operators act locally, that is, $(T_{t+h,t} f)(x)$ depends essentially upon the values of $f(y)$ with y in a small neighborhood of x. Taking into account the fact that as the scale increases, no new feature should be created by the scale space, we have the local comparison principle: if an image u is locally brighter than another image v, then this order must be conserved by the analysis. This is expressed by:

(A2) For all u and v such that $u(y) > v(y)$ in a neighborhood of x and $y \neq x$, then for h small enough, we have

$$(T_{t+h,t} u)(x) \geq (T_{t+h,t} v)(x)$$

The third assumption states that a very smooth image must evolve in a smooth way with the scale

space. Denoting the scalar product of two vectors of $\mathbb{R}^N$ by $<x,y>$, this assumption can be written as

(A3) Let $u(y) = 1/2\langle A(y-x), y-x\rangle + \langle p, y-x\rangle + c$ be a quadratic form of $\mathbb{R}^2$, x fixed ($A = \nabla^2 u(x) \in S^{(2)}$ the set of 2×2 symmetric matrices, $p = \nabla u(x)$ a vector of $\mathbb{R}^2, c = u(x)$ a constant.). We shall say that a scale space is regular if there exists a function $F(t,x,c,p,A)$, continuous with respect to A, such that

$$\frac{(T_{t+h,t}u - u)(x)}{h} \to F(t,x,c,p,A) \quad \text{when } h \to 0$$

Scale Spaces are Governed by PDEs

In the following theorem, it is stated that the former assumptions are sufficient to prove that scale spaces are in fact governed by PDEs.

Theorem 2 *Under assumptions* A1, A2, A3, *there exists a continuous function* $F: [0,T] \times \Omega \times R \times \mathbb{R}^2 \times S^{(2)} \to \mathbb{R}$ *satisfying* $F(t,x,c,p,A) \geq F(t,x,c,p,B)$ *for all* $p \in \mathbb{R}^2$, *A and B in* $S^{(2)}$ *with* $A \geq B$ *such that*

$$\delta_t(u) = \frac{T_{t+h,t}u - u}{h} \to F(t,x,u,\nabla u, \nabla^2 u), \quad h \to 0^+ \qquad [10]$$

uniformly for $x \in \mathbb{R}^2$, *uniformly for u.*

In eqn [10], the left-hand side term can be interpreted as the partial temporal derivative with respect to t so that the notion of PDEs arises. More precisely, if f is continuous and uniformly bounded, then it can be established that $u(t,x) = (T_t f)(x)$ is the viscosity solution(see Definition 3) of

$$\frac{\partial u}{\partial t} + H(t,x,u,\nabla u, \nabla^2 u) = 0 \text{ (here } H = -F) \qquad [11]$$
$$u(0,x) = f(x)$$

The map $H: [0,T] \times \Omega \times R \times R^2 \times S^{(2)} \to \mathbb{R}$ is called a Hamiltonian and the decreasing property of H with respect to S is called degenerate ellipticity.

The theory of viscosity solutions was introduced in the 1980s by Crandall and P L Lions (Crandall and Lions 1981, Crandall *et al.* 1992). When strong solutions of [11] do not exist, this theory allows to define solutions which are only continuous or even discontinuous. The definition of viscosity solutions is

Definition 3 Let $H: \Omega \times \mathbb{R} \times \mathbb{R}^2 \times S^{(2)} \to \mathbb{R}$ be continuous and degenerate elliptic and let $u \in C^0([0,T] \times \Omega)$. Then u is a viscosity solution of [11] in $[0,T] \times \Omega$ if and only if

(i) u is a subsolution, that is, $\forall \phi \in C^2([0,T] \times \Omega)$, $\forall (t_0, x_0)$ a local strict maximum point of $(u - \phi)(t,x)$, we have

$$\frac{\partial \phi}{\partial t}(t_0,x_0) + H(t_0, x_0, u(t_0,x_0), \nabla\phi(t_0,x_0), \nabla^2\phi(t_0,x_0)) \leq 0$$

(ii) u is a supersolution, that is, $\forall \phi \in C^2([0,T] \times \Omega)$, $\forall (t_0, x_0)$ a local strict minimum point of $(u - \phi)(t,x)$, we have

$$\frac{\partial \phi}{\partial t}(t_0,x_0) + H(t_0, x_0, u(t_0,x_0), \nabla\phi(t_0,x_0), \nabla^2\phi(t_0,x_0)) \geq 0$$

In this definition, it is noticeable that derivatives of u are replaced by the derivatives of the test functions ϕ. Obviously, it can be verified that this notion of weak solutions coincides with classical solution when u has enough regularity.

Diffusion Operators Coming from the Scale Space

A step further is to assume additional properties on the scale spaces and estimate the corresponding operator. Invariance properties include geometric invariance axioms, contrast invariance, or scale invariance. For example, if we assume the axioms A1–A3, gray-level shift invariance:

(I1) $T_t(0) = 0, T_t(u + c) = T_t(u) + c$ for all u and all constant c.

and translation invariance:

(I2) $T_t(\tau_h.u) = \tau_h.(T_t u)$ for all h in $\mathbb{R}^2, t \geq 0$, where $(\tau_h.u)(x) = u(x+h)$.

Then it can be established that F in [10] is independent of (x,u), that is, $u(t,x) = (T_t f)(x)$ is the unique viscosity solution of

$$\frac{\partial u}{\partial t} = F(\nabla u, \nabla^2 u)$$
$$u(0,x) = f(x)$$

With more precise assumptions, one can even recover explicitly the operator F. As an example, if we look for a linear scale space which verifies some isometry assumption:

(I3) $T_t(R.u)(x) = R.(T_t u)(x)$ for all orthogonal transformation $\mathbb{R}$ on $\mathbb{R}^2$, where $(R.u)(x) = u(Rx)$.

Then it can be proved that the scale space is the unique solution of the heat equation:

$$\begin{aligned} &\frac{\partial u}{\partial t} - \Delta u = 0 \\ &u(0,x) = f(x) \end{aligned} \qquad [12]$$

Figure 4 is an example of [12] applied to a noisy image at different scale, that is, at different time. Note that noise is quickly removed but one has to stop the evolution very early if we would like to preserve some edges. In the nonlinear cases, several operators have also been found based on curvature. For instance, under suitable axioms (Alvarez *et al.* 1993), including contrast, scale, and affine invariance, the associated scale space is

$$\begin{aligned} &\frac{\partial u}{\partial t} - \operatorname{sign}(\kappa)(t\kappa)^{1/3}|\nabla u| = 0 \\ &\quad \text{where } \kappa = \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right) \\ &u(0,x) = f(x) \end{aligned} \qquad [13]$$

This equation is called affine morphological scale space (AMSS) and three restored images are shown in **Figure 5**. Some qualitative differences are shown in **Figure 6**.



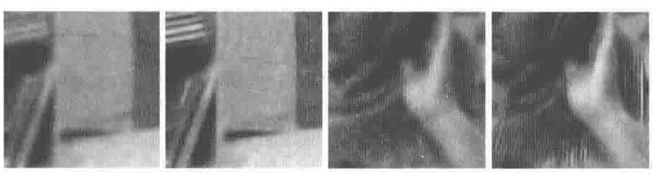
Original image 40 iterations 90 iterations 150 iterations

Figure 4 Illustration of heat equation [12].



Original image 40 iterations 90 iterations 150 iterations

Figure 5 Illustration of the AMSS model [13].



Heat AMSS Heat AMSS

Figure 6 Some close-ups of Figures 4 and 5 showing qualitative differences after 40 iterations.

Remark Scale space theory has shown the formal link between some operators and PDEs. It has to be noticed that one may propose some PDEs which do not directly come from the scale space framework. Starting from [12] which performs isotropic smoothing and smears edges, many nonlinear diffusion models have been proposed to smooth images while preserving edges (see e.g., Perona and Malik (1990)). □

To know more on scale space and PDEs, we refer the reader to Weickert (1998) and Aubert and Kornprobst (2002).

The Wavelet Approach

Before the 1980s, the Fourier transform played a major role for analyzing oscillating signals. The interest of such a transform for real application increased after the discovery of the fast Fourier transform. However, the Fourier transform has some limit. The Fourier transform extracts from the signal details of the frequency content but loses all information on the location of particular frequency. Moreover, for computing the Fourier transform $\mathcal{F}f(\lambda)$, we need to know $f(t)$ for all the real values of t. These difficulties can be overcome by first windowing the signal, and then by taking its Fourier transform:

$$\mathcal{F}^{\text{win}} f(\lambda, t) = \int_{\mathbb{R}} f(s) g(s-t) e^{-i\lambda s} ds$$

where g is a window function. The parameter λ plays the role of a frequency localized around the abscissa t of the temporal signal and $\mathcal{F}^{\text{win}} f(\lambda, t)$ give an information about what is happening around $s = t$, for the frequency λ. The main drawback of this method is that the window has a fixed length which is a serious disadvantage when we want to treat signals having variations of different orders of magnitude. All these issues highlighted that a mathematical theory of time–frequency representation was necessary. This was achieved with the wavelet representation. In this section, we first recall some elements of this theory (for 1D signal) and then we show how it can be applied for restoring noisy images.

The Wavelet Decomposition

The basic idea is to construct from a function ψ, called mother wavelet, an orthonormal basis $\{\psi_{j,k}\}$ of $L^2(\mathbb{R})$ deduced from ψ by translation and dilatation. It is required that ψ be regular, oscillating (but not too much), that ψ and $\mathcal{F}\psi$ are well localized and that ψ has some null moments. Once this function ψ is

chosen, we set $\psi_{j,k}(x) = 2^{j/2}\psi(2^jt - k), j, k \in \mathbb{Z}$. An elegant and practical way for obtaining such a basis is to construct a multiresolution analysis of $L^2(\mathbb{R})$ (Mallat 1989).

Definition 4 A multiresolution analysis of $L^2(\mathbb{R})$ is a sequence V_j, $j \in \mathbb{Z}$ of subspaces of $L^2(\mathbb{R})$, with the following properties:

(i) $\bigcap_j V_j = \{0\}$,
(ii) $V_j \subset V_{j+1}$,
(iii) $\bigcup_j V_j = L^2(\mathbb{R})$,
(iv) $f(t) \in V_j$ if and only if $f(2t) \in V_{j+1}$, and
(v) There exists a regular function ϕ with compact support such that the family $\phi(t-k), k \in \mathbb{Z}$, is an orthonormal basis of V_0 for the scalar product of $L^2(\mathbb{R})$. Such a function ϕ is called a scaling function.

Then it is straightforward to check that the family $\phi_{j,k}(t)$ defined by $\phi_{j,k}(t) = 2^{j/2}\phi(2^jt - k)$ is an orthonormal basis of V_j.

A basic example of multiresolution analysis of $L^2(\mathbb{R})$ is to choose V_0 as the set of piecewise constant functions on $\mathbb{R}$ and take ϕ as the characteristic function of the interval $[0, 1)$: $\phi(t) = \chi_{[0,1)}(t)$.

Let us now look at the link between wavelet basis and multiresolution analysis. We just give main ideas, all details can be found in the work of Mallat (1989). Assume that we have a multiresolution analysis, and let us define W_0 as the orthogonal complement of V_0 in V_1. We build the mother wavelet ψ by imposing that the family $\psi(t-k)$, $k \in \mathbb{Z}$, is an orthonormal basis of W_0. For example, if $\phi(t) = \chi_{[0,1)}(t)$, it can be shown that $\psi(t) = \chi_{[0,1/2)}(t) - \chi_{[1/2,1)}(t)$ (called the Haar wavelet). By change of scale, one gets that the family $\psi_{j,k}(t) = 2^{j/2}\psi(2^jt - k), k \in \mathbb{Z}$, is an orthonormal basis of W_j, the orthogonal complement of V_j in V_{j+1}, that is,

$$V_j \oplus W_j = V_{j+1} \qquad [14]$$

Since the V_j's are a multiresolution analysis, we have $V_J = \oplus_{j=-\infty}^{J-1} W_j$ and $L^2 = \oplus_{j=-\infty}^{j=+\infty} W_j$. It is then clear that $\psi_{j,k}(t)$ is an orthonormal basis of $L^2(\mathbb{R})$, that is, for each function $f \in L^2(\mathbb{R})$, we get the following decomposition:

$$f(t) = \sum_{-\infty}^{+\infty} \sum_k f_{j,k}\psi_{j,k}(t) \quad \text{with } f_{j,k} = \langle f, \psi_{j,k}\rangle_{L^2}$$

Let us see now how in practice a multiresolution analysis can be interpreted. Let f be a function in $L^2(\mathbb{R})$. We denote $A_{2^j}f$ (resp. $D_{2^j}f$) the operator which approximates f (resp. gives the details of f) at resolution 2^j. More precisely, $A_{2^j}f$ (resp. $D_{2^j}f$) is the projection of f on V_j (resp. on W_j):

$$A_{2^j}f(t) = \sum_{k=-\infty}^{k=+\infty} \langle f, \phi_{j,k}\rangle \phi_{j,k}(t)$$

$A_{2^j}f$ is characterized by the sequence of scalar products $A_{2^j}^d f = \{\langle f, \phi_{j,k}\rangle\}_{k\in\mathbb{Z}}$. We call $A_{2^j}^d f$ the discrete approximation of f at resolution 2^j.

In the same way, we have

$$D_{2^j}f(t) = \sum_{k=-\infty}^{k=+\infty} \langle f, \psi_{j,k}\rangle \psi_{j,k}(t)$$

$D_{2^j}f$ is characterized by the sequence of scalar products $D_{2^j}^d f = \{\langle f, \psi_{j,k}\rangle\}_{k\in\mathbb{Z}}$.

We call $D_{2^j}^d f$ the details of f at resolution 2^j. According to [14], approximation and detail are linked by the relation

$$A_{2^{j+1}}f = A_{2^j}f + D_{2^j}f$$

This means that $D_{2^j}f$ represents the details to be added to obtain from one level of approximation to the next level of approximation.

Finally, the decomposition of a signal f on a wavelet basis is obtained as an accumulation of details at scale 2^j from 0 to $+\infty$:

$$f = \sum_{j=-\infty}^{j=+\infty} D_{2^j}f = \sum_{j=-\infty}^{j=+\infty}\sum_{k=-\infty}^{k=+\infty} \langle f, \psi_{j,k}\rangle \psi_{j,k} \qquad [15]$$

Instead of considering the sum over all dyadic levels j, one can sum over $j \geq J$ for a fixed J; in this case, we have

$$f = \sum_{k=-\infty}^{k=+\infty}\sum_{j\geq J} \langle f, \psi_{j,k}\rangle \psi_{j,k} + \sum_{k=-\infty}^{k=+\infty} \langle f, \phi_{J,k}\rangle \phi_{J,k}$$

We conclude this section by showing how we can construct a 2D wavelet basis from the 1D case. We can simply use a tensor product. Scaling function and mother wavelet are given, respectively, as follows:

$$\phi(x, y) = \phi(x)\phi(y), \qquad \Psi = (\psi^1, \psi^2, \psi^3)$$

with

$$\psi^1(x, y) = \phi(x)\psi(y)$$
$$\psi^2(x, y) = \phi(y)\psi(x)$$
$$\psi^3(x, y) = \psi(x)\psi(y)$$

As for the 1D case, $A_{2^j}f$ denotes the projection of f on V_j, $D_{2^j}^1$ the horizontal details, $D_{2^j}^2$ the vertical

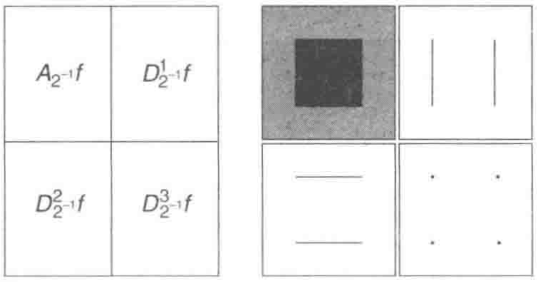


Figure 7 Illustration on the wavelets methodology.

details, and $D^3_{2^j}$ the other details (the indice l in $D^l_{2^j}$ is the same as in ψ^l). For a 2D image f, we then have the following decomposition (see **Figure** 7):

$$f = \sum_{\psi^l \in \Psi} \sum_{k=-\infty}^{k=+\infty} \sum_{j \geq J} \langle f, \psi_{j,k} \rangle \psi_{j,k} + \sum_{k=-\infty}^{k=+\infty} \langle f, \phi_{J,k} \rangle \phi_{J,k}$$

Application to the Denoising Problem

We go back to the denoising problem. Our goal is to solve this problem by using a variational approach and wavelets. We recall that we have an ideal image u that has been corrupted by a white Gaussian noise η resulting in an observation f with $f = u + \eta$. As it has been seen in the section "The variational approach," this question can be tackled by solving the variational problem

$$\min_u \{\lambda \phi(|u|_E) + |f - u|_G\} \qquad [16]$$

for suitable choices of E, G, and ϕ. Here we propose to choose $G = L^2(\Omega)$ (Ω is the domain image) and for E the Besov space $B^1_1(L^1(\Omega))$ and $\phi =$ Identity. Besov spaces $B^\alpha_q(L^p(\Omega))$ are used in many domains of mathematics as harmonic analysis or approximation theory. There exist different ways for defining them. Roughly speaking, they consist of functions having α derivatives in $L^p(\Omega)$; the third parameter q allows one to make finer distinctions in smoothness. Here we are only concerned with the Besov space $B^1_1(L^1(\Omega))$. One important property needed here is that the norm of a function in $E = B^1_1(L^1(\Omega))$ is equivalent to the l^1-norm of the wavelet coefficients, that is if $\{\psi_{j,k}\}$ is an orthonormal basis of $L^2(\Omega)$ and if $u_{j,k,\psi}$ are the wavelet coefficients of $u \in E$, then $|u|_E = \sum_j \sum_{k,\psi} |u_{j,k,\psi}|$.

Remark When one is concerned with a finite domain, then some changes must be made with respect to the construction given in [15] to obtain an orthonormal basis of $L^2(\Omega)$. To avoid further technical complications, we ignore this question. □



Original noisy image BV regularization Wavelet shrinkage

Figure 8 Illustration of two regularization methods.

Let us denote, respectively, by $\{u_{j,k,\psi}\}$ and $\{f_{j,k,\psi}\}$ the wavelet coefficients of u and f, then solving [16] amounts to finding the minimizer of the functional

$$F(u) = \lambda \sum_{j,k,\psi} |u_{j,k,\psi}| + \sum_{j,k,\psi} |u_{j,k,\psi} - f_{j,k,\psi}|^2 \qquad [17]$$

One notes immediately that minimizing problem [17] reduces to finding the minimizer s, given t, of $E(s) = |s - t|^2 + \lambda|s|$ and that the minimizer of $E(s)$ is given by $s = t - (\lambda/2)$ if $t > \lambda/2, s = 0$ if $|t| \leq \lambda/2$ and $s = t + (\lambda/2)$ if $t < -(\lambda/2)$.

Thus, we shrink the wavelet coefficients $f_{j,k,\psi}$ toward zero by an amount of $\lambda/2$ to obtain the minimizer. This is exactly the wavelet shrinkage algorithm of Donoho and Johnstone (1994). It is remarkable that the wavelet shrinkage algorithm, which has been found by using statistical tools, can also be explained via a variational approach (Chambolle *et al.* 1998). **Figure** 8 shows an example of the result on a noisy image.

For more details, we refer the reader to Mallat (1998).

Conclusion

Image processing is a challenging domain of applied mathematics which has to deal with discrete and continuous representations. In this article, we have covered the core mathematical tools used in the area. The example of gray-scale image restoration allowed us to illustrate and compare the different methodologies. Naturally, as mentioned in the introduction, image processing refers to a wide variety of applications and an intensive research has been carried out on the different topics using the methodologies described here. The reader will find in the references (therein) several illustrations of challenging problems.

See also: Γ-Convergence and Homogenization; Convex Analysis and Duality Methods; Elliptic Differential

Equations: Linear Theory; Evolution Equations: Linear and Nonlinear; Fluid Mechanics: Numerical Methods; Fractal Dimensions in Dynamics; Free Interfaces and Free Discontinuities: Variational Problems; Geometric Measure Theory; Ginzburg–Landau Equation; Inequalities in Sobolev Spaces; Minimax Principle in the Calculus of Variations; Optimal Transportation; Partial Differential Equations: Some Examples; Stochastic Differential Equations; Variational Techniques for Ginzburg–Landau Energies; Wavelets: Applications; Wavelets: Mathematical Theory.

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Incompressible Euler Equations: Mathematical Theory

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Introduction

In this article we present comprehensive mathematical results on the incompressible Euler equations. Our presentation is focussed on the two aspects of the equations. The first one is on the theories of classical solutions and the problem of global in time continuation/finite time blow-up of the local classical solutions. The second topic is concerned on the weak solutions, mainly for the two-dimensional (2D) Euler equations for existence and uniqueness questions.

The motion of homogeneous incompressible ideal fluid in a domain $\Omega \subset \mathbb{R}^n$ is described by the following system of Euler equations:

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla p \qquad [1]$$

$$\operatorname{div} v = 0 \qquad [2]$$

$$v(x,0) = v_0(x) \qquad [3]$$

where $v = (v^1, v^2, \ldots, v^n), v^j = v^j(x,t), j = 1, 2, \ldots, n$, is the velocity of the fluid flows, $p = p(x,t)$ is the scalar pressure, and $v_0(x)$ is a given initial velocity field satisfying $\operatorname{div} v_0 = 0$. Here we use the standard notion of vector calculus, denoting

$$\nabla p = \left(\frac{\partial p}{\partial x_1}, \frac{\partial p}{\partial x_2}, \ldots, \frac{\partial p}{\partial x_n}\right)$$

$$(v \cdot \nabla)v^j = \sum_{k=1}^{n} v^k \frac{\partial v^j}{\partial x_k}$$

$$\operatorname{div} v = \sum_{k=1}^{n} \frac{\partial v^k}{\partial x_k}$$

Equation [1] represents the balance of momentum for each portion of fluid, while eqn [2] represents the conservation of mass of fluid during its motion, combined with the homogeneity (constant density) assumption on the fluid. Equations [1] and [2] are first obtained by Euler in 1755. Although we could consider, more generally, the inhomogeneous incompressible Euler equations, in mathematical fluid mechanics considerations the incompressible Euler equations usually mean the above system [1]–[2]. For a bounded domain with fixed boundary $\partial\Omega$, the natural boundary condition is

$$v(x,t) \cdot \nu(x) = 0 \quad \forall (x,t) \in \partial\Omega \times [0,\infty) \qquad [4]$$

where $\nu(x)$ is the unit normal vector at the boundary point $x \in \partial\Omega$. Several studies are concerned with the Cauchy problem of the system [1]–[3], where we consider the case

$$\Omega = \begin{cases} \mathbb{R}^n (\text{whole domain of } \mathbb{R}^n), \text{or} \\ \mathbb{R}^n/\mathbb{Z}^n (\text{periodic domain}) \end{cases} \qquad [5]$$

In this article for simplicity we suppose $\Omega = \mathbb{R}^n, n = 2,3$ unless otherwise stated. We note that the Euler equation is obtained formally by setting the viscosity $= 0$, or, equivalently, Reynolds number $= \infty$ in the Navier–Stokes equations. Thus, we may view the Euler equations as the one describing approximately the extremely high Reynolds number turbulent flows. For detailed mathematical studies on the finite Reynolds number Navier–Stokes equations, see Temam (1984) and Lions (1996). For much shorter and more comprehensive review see Constantin (1995). In the study of the Euler equations the notion of vorticity, $\omega = \operatorname{curl} v$, plays a very important role. In particular, we can reformulate the system in terms of vorticity fields only as follows. We first suppose we are working in three-dimensional (3D) space, and rewrite [1] as

$$\frac{\partial v}{\partial t} - v \times \operatorname{curl} v = -\nabla\left(p + \frac{1}{2}|v|^2\right) \qquad [6]$$

Taking curl of [6], and using elementary vector identities we obtain the following vorticity formulation:

$$\frac{\partial \omega}{\partial t} + (v \cdot \nabla)\omega = \omega \cdot \nabla v \qquad [7]$$

$$\operatorname{div} v = 0, \qquad \operatorname{curl} v = \omega \qquad [8]$$

$$\omega(x,0) = \omega_0(x) \qquad [9]$$

The linear elliptic system [8] for v can be solved explicitly in terms of ω to give the Biot–Savart law

$$v(x,t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{(x-y) \times \omega(y,t)}{|x-y|^3} \, dy \qquad [10]$$

Substituting this v into [7] formally, we obtain a integrodifferential system for ω. The term in the right-hand side of [7] is called the "vortex stretching term," and is regarded as the main source of difficulties in the mathematical theory of the 3D Euler equations. In the 2D case we take the vorticity as the scalar, $\omega = \partial v^2/\partial x_1 - \partial v^1/\partial x_2$, and the evolution equation of ω becomes

$$\frac{\partial \omega}{\partial t} + (v \cdot \nabla)\omega = 0 \qquad [11]$$

combined with the 2D Biot–Savart law,

$$v(x,t) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{(-y_2 + x_2, y_1 - x_1)}{|x-y|^2} \omega(y,t) \, dy \qquad [12]$$

In many studies of the Euler equations it is convenient to introduce the notion of "particle trajectory mapping," $\Phi(\cdot,t)$ defined by

$$\frac{\partial \Phi(\alpha,t)}{\partial t} = v(\Phi(\alpha,t),t)$$
$$\Phi(\alpha,0) = \alpha, \qquad \alpha \in \Omega \qquad [13]$$

The mapping $\Phi(\cdot,t)$ transforms from the location of the initial fluid particles to the location at time t, and the parameter α is called the Lagrangian particle marker. If we denote the Jacobian of the transformation, $\det(\nabla_\alpha \Phi(\alpha,t)) = J(\alpha,t)$, then we can show easily that

$$\frac{\partial J}{\partial t} = (\operatorname{div} v) J$$

which implies the fact that the velocity field v satisfies the incompressibility, $\operatorname{div} v = 0$ if and only if the mapping $\Phi(\cdot,t)$ is volume preserving. At this moment, we note that, although the Euler equations are originally derived by applying the mass conservation and the momentum balance principles, we could also derive them by applying the principle of least action to the action defined by

$$\mathcal{A}(\Phi) = \frac{1}{2} \int_{t_1}^{t_2} \int_\Omega \left| \frac{\partial \Phi(x,t)}{\partial t} \right|^2 dx \, dt$$

Here, $\Phi(\cdot,t) : \Omega \to \Omega$ is a parametrized family of volume-preserving diffeomorphism. This variational approach to the Euler equations implies that we can

view solutions of the Euler equations as a geodesic curve in the L^2-metric on the infinite-dimensional manifold of volume-preserving diffeomorphisms (see for more details, e.g., Arnol'd and Khesin (1998)).

The 3D Euler equations have many conserved quantities. We list some important ones below.

1. *Energy*

$$E(t) = \frac{1}{2}\int_\Omega |v(x,t)|^2\,dx \qquad [14]$$

2. *Helicity*

$$H(t) = \int_\Omega v(x,t)\cdot\omega(x,t)\,dx \qquad [15]$$

3. *Circulation*

$$\Gamma_{C(t)} = \oint_{C(t)} v\cdot dl \qquad [16]$$

where $C(t)=\{\Phi(\alpha,t)|\alpha\in C\}$ is the curve moving along with the fluid.

4. *Impulse*

$$I(t) = \frac{1}{2}\int_\Omega x\times\omega\,dx \qquad [17]$$

5. *Moment of impulse*

$$M(t) = \frac{1}{3}\int_\Omega x\times(x\times\omega)\,dx \qquad [18]$$

The proof of conservations of the above quantities can be carried out without difficulty by using elementary vector calculus (for details see, e.g., Chorin and Marsden (1993), Majda and Bertozzi (2002), Marchioro and Pulvirenti (1994)). The helicity above, in particular, represents the degree of knotedness of the vortex lines in the fluid, where the vortex lines are the integral curves of the vorticity fields. Arnol'd and Khesin (1998) discuss in detail aspects of helicity and other geometric aspects of the Euler equations. For the 2D Euler equations there is no analog of helicity, while the circulation conservation is replaced by the vorticity flux integral,

$$\int_{A(t)} \omega(x,t)\,dx \qquad [19]$$

where $A(t)=\{\Phi(\alpha,t)|\alpha\in A\}$ is a planar region moving along the fluid. The impulse and the moment of impulse integrals are replace by

$$\frac{1}{2}\int_\Omega (x_2,-x_1)\omega\,dx \qquad [20a]$$

and

$$-\frac{1}{3}\int_\Omega |x|^2\omega\,dx \qquad [20b]$$

respectively.

In the 2D ideal incompressible fluids we have extra conserved quantities; namely for any $p\in[1,\infty]$ the integral

$$\int_\Omega |\omega(x,t)|^p dx \qquad [21]$$

is conserved (as a matter of fact we can extend this statement by replacing the integral by $\int_\Omega f(\omega(x,t))dx$ for any continuous function f). There are many known explicit solutions to the Euler equations (See e.g., Lamb (1932) and Majda and Bertozzi (2002)).

Local Existence and the Blow-Up Problem

The Classical Results

We first introduce some notations of function spaces. The Lebesgue space $L^p(\Omega), p\in[1,\infty]$, is the Banach space defined by the norm

$$\|f\|_{L^p} := \begin{cases} \left(\int_\Omega |f(x)|^p dx\right)^{1/p}, & p\in[1,\infty) \\ \text{ess.}\sup_{x\in\Omega}|f(x)|, & p=\infty \end{cases}$$

Let us set $\alpha:=(\alpha_1,\alpha_2,\ldots,\alpha_n)\in(\mathbb{Z}_+\cup\{0\})^n$ with $|\alpha|=\alpha_1+\alpha_2+\cdots+\alpha_n$. Then, $D^\alpha:=D_1^{\alpha_1}D_2^{\alpha_2}\cdots D_n^{\alpha_n}$, where $D_j=\partial/\partial x_j, j=1,2,\ldots,n$. For given $k\in\mathbb{Z}$ and $p\in[1,\infty)$ the Sobolev space, $W^{k,p}(\Omega)$ is the Banach space of functions consisting of functions $f\in L^p(\Omega)$ such that

$$\|f\|_{W^{k,p}} := \left(\int_\Omega |D^\alpha f(x)|^p\,dx\right)^{1/p} < \infty$$

where the derivatives are in the sense of distributions. For $p=\infty$ we replace the L^p-norm by the L^∞ norm. In order to cooperate with the fractional derivatives of order $s\in\mathbb{R}$, we use the space $L_p^s(\Omega)$ defined by the Banach spaces norm,

$$\|f\|_{L^{s,p}} := \|(1-\Delta)^{s/2}f\|_{L^p}$$

where $(1-\Delta)^{s/2}f=\mathcal{F}^{-1}[(1+|\xi|^2)^{s/2}\mathcal{F}(f)(\xi)]$ with $\mathcal{F}(\cdot)$ and $\mathcal{F}^{-1}(\cdot)$ denoting the Fourier transform and its inverse. Below we outline the key ideas of proving the local existence theorems for the Euler equations. For more details we refer the reader to Majda and Bertozzi (2002). For simplicity, we use the function space $H^m(\mathbb{R}^n)=W^{m,2}(\mathbb{R}^n), n=2,3$. Taking derivatives D^α on [1], and then taking its

L^2 inner product with $D^\alpha v$, and summing over the multi-indices α with $|\alpha| \le m$, we obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|v\|_{H^m}^2 &= -\sum_{|\alpha|\le m}(D^\alpha(v\cdot\nabla)v-(v\cdot\nabla)D^\alpha v, D^\alpha v)_{L^2}\\ &\quad-\sum_{|\alpha|\le m}((v\cdot\nabla)D^\alpha v, D^\alpha v)_{L^2}\\ &\quad-\sum_{|\alpha|\le m}(D^\alpha\nabla p, D^\alpha v)_{L^2}\\ &\equiv \mathrm{I}+\mathrm{II}+\mathrm{III}\end{aligned}$$

By integration by parts, we obtain

$$\mathrm{III} = -\sum_{|\alpha|\le m}(D^\alpha p, D^\alpha \operatorname{div} v)_{L^2} = 0$$

Integrating by parts again, and using the fact that div $v=0$, we have

$$\begin{aligned}\mathrm{II} &= -\frac{1}{2}\sum_{|\alpha|\le m}\int_{\mathbb{R}^3}(v\cdot\nabla)|D^\alpha v|^2\,\mathrm{d}x\\ &=\frac{1}{2}\sum_{|\alpha|\le m}\int_{\mathbb{R}^3}\operatorname{div} v|D^\alpha v|^2\,\mathrm{d}x = 0\end{aligned}$$

We now use the so-called commutator type of estimate,

$$\begin{aligned}&\sum_{|\alpha|\le m}\|D^\alpha(fg)-fD^\alpha g\|_{L^2}\\ &\quad\le C(\|\nabla f\|_{L^\infty}\|g\|_{H^{m-1}}+\|f\|_{H^m}\|g\|_{L^\infty})\end{aligned}$$

and obtain

$$\begin{aligned}I &\le \sum_{|\alpha|\le m}\|D^\alpha(v\cdot\nabla)v-(v\cdot\nabla)D^\alpha v\|_{L^2}\|v\|_{H^m}\\ &\le C\|\nabla v\|_{L^\infty}\|v\|_{H^m}^2\end{aligned}$$

Summarizing the above estimates, I–III, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\|v\|_{H^m}^2 \le C\|\nabla v\|_{L^\infty}\|v\|_{H^m}^2 \qquad [22]$$

Further estimate, using the Sobolev inequality, $\|\nabla v\|_{L^\infty} \le C\|v\|_{H^m}$ for $m > 5/2$, gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\|v\|_{H^m}^2 \le C\|v\|_{H^m}^3$$

Thanks to Gronwall's lemma, we have the local-in-time uniform estimate

$$\|v(t)\|_{H^m} \le \frac{\|v_0\|_{H^m}}{1-Ct\|v_0\|_{H^m}} \le 2\|v_0\|_{H^m}$$

for all $t \in [0, 1/(2C\|v_0\|_{H^m})]$. This is the key *a priori* estimate for the construction of the local solutions. The local-in-time solution of the Euler equations in the Sobolev space $H^m(\mathbb{R}^n)$ for $m > n/2+1, m \in \mathbb{Z}$, was obtained by Kato (1972). For the above-constructed local-in-time solutions, one of the most outstanding open problems in mathematical fluid mechanics is whether the solution can be continued to any future time up to infinity, or the solution will lose regularity and blow up in finite time. Even in terms of numerical experiments, the answer is not yet settled down. In the direction of solving this problem there is a celebrated results, called the Beale–Kato–Majda criterion (1984), which states

$$\limsup_{t\nearrow T_*}\|v(t)\|_{H^s}=\infty \quad \text{if and only if} \quad \int_0^{T_*}\|\omega(s)\|_{L^\infty}ds=\infty \qquad [23]$$

We outline the proof of this result below (for more details see Majda and Bertozzi (2002)). We first recall the Beale–Kato–Majda's version of the logarithmic Sobolev inequality,

$$\|\nabla v\|_{L^\infty} \le C\|\omega\|_{L^\infty}(1+\log(1+\|v\|_{H^m}))+C\|\omega\|_{L^2} \qquad [24]$$

for $m > 5/2$. Now suppose $\int_0^{T_*}\|\omega(t)\|_{L^\infty}\mathrm{d}t < \infty$. Taking L^2 inner product of [7] with ω, then after integration by part we obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\omega\|_{L^2}^2 &= ((\omega\cdot\nabla)v,\omega)_{L^2}\\ &\le \|\omega\|_{L^\infty}\|\nabla v\|_{L^2}\|\omega\|_{L^2}\\ &= \|\omega\|_{L^\infty}\|\omega\|_{L^2}^2\end{aligned}$$

where we used the identity $\|\nabla v\|_{L^2} = \|\omega\|_{L^2}$. Applying the Gronwall lemma, we obtain

$$\begin{aligned}\|\omega(t)\|_{L^2} &\le \|\omega_0\|_{L^2}\exp\left(\int_0^{T_*}\|\omega(s)\|_{L^\infty}\,\mathrm{d}s\right)\\ &\le C(\omega_0, T_*)\end{aligned} \qquad [25]$$

for all $t \in [0, T_*]$. Substituting [24] into [22], and combining this with [25], we have

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\|v\|_{H^m}^2\\ &\quad\le C[1+\|\omega\|_{L^\infty}[1+\log(1+\|v\|_{H^m})]]\|v\|_{H^m}^2\end{aligned}$$

Applying the Gronwall's lemma, we obtain

$$\begin{aligned}\|v(t)\|_{H^m} &\le \|v_0\|_{H^m}\\ &\quad\times\exp\left[C_1\exp\left(C_2\int_0^{T_*}\|\omega(\tau)\|_{L^\infty}\,\mathrm{d}\tau\right)\right]\\ &\le C(v_0, T_*)\end{aligned}$$

for all $t \in [0, T_*]$ and for some constants C_1, C_2. Thus, we proved the "necessity part" of [23], The

"sufficiency part" is an easy consequence of the Sobolev inequality,

$$\int_0^{T_*} \|\omega(s)\|_{L^\infty}\, ds \leq T_* \sup_{0\leq t\leq T_*} \|\nabla v(t)\|_{L^\infty} \leq CT_* \sup_{0\leq t\leq T_*} \|v(t)\|_{H^m}$$

for $m > 5/2$.

Other Related Results

The previous local existence result in $H^m(\mathbb{R}^n), m > n/2+1$, is basically due to T Kato in 1972. He and G Ponce extended this existence result using the fractional Sobolev space, $L_p^s(\mathbb{R}^n), s > n/2+1, s \in \mathbb{R}$ in 1986. These results were further extended, using the Besov and the Triebel–Lizorkin spaces, by the present author in 2001.

For bounded domain $\Omega \subset \mathbb{R}^n$, R Temam obtained the local-existence result using the space $W^{k,p}(\Omega)$ in 1975. On the other hand, in the setting of the Hölder space, $C^{1,\alpha}(\mathbb{R}^n)$ L Lichtenstein (1925) and W Wolibner (1933) obtained local existence of solutions of the Euler equations. More recently, J-Y Chemin considered the Zygmund $C^s(\mathbb{R}^n)$, which is identical to the Hölder space $C^{[s],s-[s]}(\mathbb{R}^n)$ for noninteger s, where $[s]$ means the largest integer not greater than s, but is different from $C^{[s],0}(\mathbb{R}^n)$ for integer s. He proved, in 1992, local existence of solutions to the 3D Euler equations in this space in 1992. See Chemin (1998) for details of this proof.

The Beale–Kato–Majda criterion for the finite-time blow-up of the classical solutions of the 3D Euler equations has been refined recently by many authors; replacing the L^∞-norm of vorticity $\omega(x,t)$ by the weaker BMO (the space of functions with bounded mean oscillations) norm (H Kozono and Y Taniuchi, 2000), and by the even weaker Besov space or Triebel–Lizorkin space norms by the present author in 2001 (see Triebel (1983) for more details on those spaces). Here we just note that these spaces are refinements of the usual Sobolev spaces. For a bounded domain case, there is a result by A Ferrari in 1993. The blow-up problem is still open even in the case of axisymmetric 3D Euler equations if there is a nonzero swirl (angular velocity). In this case, the blow-up is controlled only by the angular component of the vorticity as shown by the present author (1996). In the region off the axis, in particular, the axisymmetric 3D Euler equation has the same form as the 2D Boussinesq equations.

Some researchers also tried to approach to regularity/singularity problem of the 3D Euler equations by investigating the geometric structure of the vortex stretching term, and obtained a geometric type of blow-up criterion (P Constantin, C Fefferman, and A Majda, 1996). For more detailed review of studies in this direction see Constantin (1995).

Since the blow-up problem of the 3D Euler equation itself looks too difficult to solve, it has also been studied on the simplified model problems. In 1985, P Constantin, PD Lax, and A Majda considered the following 1D model problem of the 3D Euler equations:

$$\theta_t + (H(\theta)\theta)_x = 0, \quad \theta(x,0) = \theta_0(x)$$

where $H(\cdot)$ is the Hilbert transform defined by

$$H(\omega) = \frac{1}{\pi} PV \int_{-\infty}^{\infty} \frac{\omega(y)}{x-y}\, dy$$

They proved finite-time blow-up of this model problem by explicitly obtaining the solution. There is another, 2D model problem of the 3D Euler equations, the quasigeostrophic equations,

$$\begin{gathered}\theta_t + (u\cdot\nabla)\theta = 0 \\ u = \nabla^\perp\psi, \qquad \theta = -(-\Delta)^{1/2}\psi \\ \theta(x,0) = \theta_0(x)\end{gathered} \qquad [26]$$

where $\nabla^\perp = (-\partial_2, \partial_1)$. Contrary to the above 1D model equation, this 2D model has real physical relevance in the atmospheric science, and $\theta(x,t)$ represents the temperature of the air. The resemblance of this equation to the 3D Euler equation was first observed by P Constantin, A Majda, and E Tabak in 1994, and they derived the finite blow-up criterion of the equations. In spite of many interesting partial results, including the work by D Cordoba (1998), the blow-up problem of [26] is still open.

The 2D Euler Equations and the Weak Solutions

The Case of $W^{1,p}$ Weak Solutions

In 2D Euler equations, the problem of global well-posedness of the classical solutions is settled down. This is an immediate consequence of the conservation of $\|\omega(t)\|_{L^\infty}$ as stated in [21] combined with the Beale–Kato–Majda criterion [23]. On the other hand, the notion of weak solutions is not well understood. A weak solution of the Euler equations is a singular (nondifferentiable) solution of the equations. More precisely, by a weak solution of

[1]–[2] in $\Omega \times (0,T)$ we mean a vector field $v \in C([0,T); L^2_{\text{loc}}(\Omega))$ satisfying the integral identity:

$$-\int_0^T \int_{\mathbb{R}^3} v(x,t) \cdot \frac{\partial \phi(x,t)}{\partial t} \, dx \, dt - \int_{\mathbb{R}^3} v(x,0) \cdot \phi(x,0) \, dx - \int_0^T \int_{\mathbb{R}^3} v(x,t) \otimes v(x,t) : \nabla \phi(x,t) \, dx \, dt = 0 \quad [27a]$$

$$\int_0^T \int_{\mathbb{R}^3} v(x,t) \cdot \nabla \psi(x,t) \, dx \, dt = 0 \quad [27b]$$

for every vector test function $\phi = (\phi_1, \phi_2, \ldots, \phi_n) \in C_0^\infty(\Omega \times [0,T))$ satisfying div $\phi = 0$, and for every scalar test function $\psi \in C_0^\infty(\Omega \times [0,T))$. Here we used the notation $(u \otimes v)_{ij} = u_i v_j$, and $A:B = \sum_{i,j=1}^n A_{ij} B_{ij}$ for $n \times n$ matrices A and B. We observe that [27a] and [27b] are obtained by multiplying ϕ and ψ to [1] and [2], respectively, and integrating by parts. Thus, even the locally square-integrable vector fields, which are not differentiable in the classical sense, could be solutions of the Euler equations. For the general 3D Euler equations, we do not yet have the global existence theorems for the weak solutions. Actually, it is even suggested that we need more weaker notion of solution (the so-called "measure-valued solutions") to describe generic global solutions for the 3D Euler equations. For the 2D Euler equations, however, we have global existence theorems for $\omega_0 \in L^1(\mathbb{R}^2) \cap L^p(\mathbb{R}^2)$ for $p \in [1, \infty]$. This better situation of 2D Euler equations compared to the 3D case for the weak solutions is mainly due to the conservation law of L^p-norm described in [21]. Here we present briefly the existence proof of the weak solutions for 2D Euler equations in the simplest situation. We will prove the global existence of weak solutions for $\omega_0 \in L^p(\mathbb{R}^2), 1 < p < \infty$. Let $\rho_\varepsilon(x) = (1/\varepsilon^2)\rho(x/\varepsilon)$, where $\rho \in C_0^\infty(\mathbb{R}^2)$ is a standard mollifier, satisfying $\rho \geq 0$, supp $\rho \subset \{x \in \mathbb{R}^2 | |x| < 1\}$, and $\int_{\mathbb{R}^2} \rho \, dx = 1$. Let v_0 be the velocity associated with the initial vorticity ω_0, given by the Biot–Savart law [12]. Define the sequence of initial data $v_0^\varepsilon(x) = \rho_\varepsilon * v_0(x) = \int_{\mathbb{R}^2} \rho_\varepsilon(x-y) v_0(y) \, dy$. For each v_0^ε we have global-in-time smooth solutions $v^\varepsilon(x,t)$. Moreover, thanks to [21], we have the following estimate of the vorticity that is uniform in ε:

$$\|\omega(t)^\varepsilon\|_{L^p} = \|\omega_0^\varepsilon\|_{L^p} \leq \|\omega_0\|_{L^p} \quad [28]$$

where we used the property of the mollifier in the second inequality. If we take the (distributional) derivative of the Biot–Savart law [12], we find $\nabla v = K * \omega + C\omega$, where $K(x)$ is a kernel function defining a singular integral operator of the convolution type, and C is a constant vector. The well-known Calderon–Zygmund inequality implies that

$$\|\nabla v\|_{L^p} \leq C_p \|\omega\|_{L^p} \quad [29]$$

Combining [28] and [29] we have

$$\sup_{0 \leq t \leq T} \|\nabla v^\varepsilon(t)\|_{L^p} \leq C(v_0), \quad \forall T > 0 \quad [30]$$

namely the sequence $\{v^\varepsilon\}$ is uniformly bounded in $L^\infty(0,T; W^{1,p}(\mathbb{R}^2))$. Next, we claim that $\{v^\varepsilon\}$ satisfies the inequality

$$\|v^\varepsilon(t_1) - v^\varepsilon(t_2)\|_{H^{-3}(\mathbb{R}^2)} \leq C\|v_0\|_2^2 |t_1 - t_2| \quad [31]$$

for all t_1, t_2 with $0 < t_1 \leq t_2 < T$, where C is an absolute constant. Here the negative-order Sobolev space $H^{-m}(\Omega), m > 0$, is defined as the dual of $H_0^m(\Omega)$, and can be identified with the space of functions $C_0^\infty(\Omega)$ completed with metric in $H^m(\Omega)$. Indeed, let $\phi \in C_0^\infty(\mathbb{R}^2)$. Taking $L^2(\mathbb{R}^2)$ inner product of [1] with ϕ we have the estimates

$$\begin{aligned}
\left| \int_{\mathbb{R}^2} \frac{\partial v^\varepsilon(x,t)}{\partial t} \cdot \phi(x) \, dx \right|
&\leq \left| \int_{\mathbb{R}^2} (\phi \cdot \nabla) p^\varepsilon \, dx \right| + \left| \int_{\mathbb{R}^2} \phi \cdot (v^\varepsilon \cdot \nabla) v^\varepsilon \, dx \right| \\
&= \left| \int_{\mathbb{R}^2} p^\varepsilon \nabla \phi \, dx \right| + \left| \int_{\mathbb{R}^2} (v^\varepsilon \cdot \nabla) \phi v^\varepsilon \, dx \right| \\
&\leq \|p^\varepsilon(t)\|_{H^{-2}} \|\nabla \phi\|_{H^2} + \|v^\varepsilon(t)\|_{L^2}^2 \|\nabla \phi\|_\infty \\
&\leq C(\|p^\varepsilon(t)\|_{H^{-2}} + \|v_0^\varepsilon\|_{L^2}^2) \|\phi\|_{H^3}
\end{aligned} \quad [32]$$

where we used the Sobolev inequality $\|\nabla \phi\|_{L^\infty} \leq C\|\phi\|_{H^3}$ and the energy equality in the last step. Since [32] holds for all $\phi \in C_0^\infty(\mathbb{R}^2)$, by taking the closure of $C_0^\infty(\mathbb{R}^2)$ in $H^3(\mathbb{R}^2)$ we obtain

$$\left\| \frac{dv^\varepsilon(t)}{dt} \right\|_{H^{-2}} \leq C\|p^\varepsilon(t)\|_{H^{-2}} + \|v_0\|_{L^2}^2 \quad [33]$$

We now estimate $\|p^\varepsilon(t)\|_{H^{-2}}$. Taking the divergence operation on [1], we have the Poisson equation

$$\Delta p^\varepsilon = -\text{div}(v^\varepsilon \cdot \nabla v^\varepsilon)$$

Let $\eta \in C_0^\infty(\mathbb{R}^2)$, then

$$\begin{aligned}
\left| \int_{\mathbb{R}^2} \Delta p^\varepsilon(x,t) \eta(x) \, dx \right| &= \left| \int_{\mathbb{R}^2} \text{div}(v^\varepsilon \cdot \nabla v^\varepsilon) \eta \, dx \right| \\
&= \left| \int_{\mathbb{R}^2} (v^\varepsilon \cdot \nabla) v^\varepsilon \cdot \nabla \eta \, dx \right| \\
&= \left| \int_{\mathbb{R}^2} (v^\varepsilon \cdot \nabla) \nabla \eta \cdot v^\varepsilon \, dx \right| \\
&\leq \|v^\varepsilon(t)\|_{L^2}^2 \|\Delta^2 \eta\|_{L^\infty} \\
&\leq C\|v_0\|_{L^2}^2 \|\eta\|_{H^4}
\end{aligned} \quad [34]$$

where we used the energy equality [14] and the Sobolev inequality in the last step. Since [34] holds for all $\eta \in C_0^\infty(\mathbb{R}^2)$, taking the closure of $C_0^\infty(\mathbb{R}^2)$ in $H^4(\mathbb{R}^2)$, we obtain

$$\left|\int_{\mathbb{R}^2} \Delta p^\varepsilon(x,t)\eta(x)\,dx\right| \le C\|v_0\|_{L^2}^2\|\eta\|_{H^4} \quad \forall \eta \in H^4(\mathbb{R}^2) \qquad [35]$$

Thus,

$$\|\Delta p^\varepsilon(t)\|_{H^{-4}} \le C\|v_0\|_{L^2}^2 \quad \forall t \in [0,T)$$

This provides us with

$$\|p^\varepsilon(t)\|_{H^{-2}} \le \|D^2 p^\varepsilon(t)\|_{H^{-4}} \le C\|\Delta p^\varepsilon(t)\|_{H^{-4}} \le C\|v_0\|_{L^2}^2$$

Combining [33] with [36], we obtain

$$\sup_{0\le t\le T}\left\|\frac{dv^\varepsilon(t)}{dt}\right\|_{H^{-2}} \le C\|v_0\|_{L^2}^2$$

Thus, from

$$v^\varepsilon(t_1) - v^\varepsilon(t_2) = \int_{t_2}^{t_1} \frac{dv^\varepsilon(t)}{dt}\,dt$$

we have

$$\|v^\varepsilon(t_1) - v^\varepsilon(t_2)\|_{H^{-2}} \le \sup_{0\le t\le T}\left\|\frac{dv^\varepsilon(t)}{dt}\right\|_{H^{-2}}|t_1 - t_2| \le C\|v_0\|_{L^2}^2|t_1 - t_2|$$

Thus, [31] is proved as claimed. Thanks to the Aubin–Nitsche compactness lemma together with [30] and [31] we have a subsequence, denoted by the same notation, $\{v^\varepsilon\}$ and v in $L^\infty(0,T;W^{1,p}(\mathbb{R}^2))$ such that

$$v^\varepsilon \to v \text{ weakly} - * \text{ in } L^\infty(0,T;W^{1,p}(\mathbb{R}^2)) \qquad [36]$$

and

$$v^\varepsilon \to v \quad \text{in } L^2_{\mathrm{loc}}(\mathbb{R}^2 \times (0,T)) \qquad [37]$$

as $\varepsilon \to 0$. We know that as a classical solution each v^ε and v_0^ε satisfies

$$\int_{\mathbb{R}^2} \phi(x,0)v_0^\varepsilon(x)dx + \int_0^T\int_{\mathbb{R}^2} (\phi_t \cdot v^\varepsilon + \nabla\phi : v^\varepsilon \otimes v^\varepsilon)\,dx\,dt = 0 \qquad [38]$$

for all $\phi \in C_0^\infty(\mathbb{R}^2 \times [0,T))$ with $\operatorname{div}\phi = 0$ and

$$\int_0^T\int_{\mathbb{R}^2} \nabla\psi \cdot v^\varepsilon\,dx\,dt = 0 \qquad [39]$$

for all $\psi \in C_0^\infty(\mathbb{R}^2 \times [0,T))$. We can check easily that the convergence [36] and [37] is enough to pass to the limit $\varepsilon \to 0$ in [38] and [39] to obtain the corresponding equations with v^ε and v_0^ε replaced by v and v_0. Thus, v is a weak solution of the Euler equations with initial data v_0. This completes the outline of the proof of weak solutions to the 2D Euler equations.

Notes on Further Results

The study of weak solutions of the 2D Euler equations was initiated by V Yudovich in 1963, where he proved the existence of weak solutions for initial data $\omega_0 \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$. Subsequenthy, theory of weak solutions has been developed by studies of the vortex sheet problem due to DiPerna and Majda in 1987. For the existence of weak solutions to the vortex sheet initial data, namely the existence problem for initial vorticity $\omega_0 \in H^{-1}(\mathbb{R}^2) \cap \mathcal{M}(\mathbb{R}^2)$, where $\mathcal{M}(\mathbb{R}^2)$ is the space of Radon measures on $\mathbb{R}^2$, is still an outstanding open problem. The main physical motivation of this problem is to understand the dynamics of vortex sheets in the 3D turbulence. For this problem JM Delort proved existence assuming single-signedness of the initial vortex sheet in 1991. The proof is simplified by A Majda in 1993, using the conservation of moment of impulse. The result is also reproved by LC Evans and S Müller in 1994, using the weak compactness of the Hardy space. Later in 2001, MC Lopes Filho, HJ Nussenzveig Lopes and Z Xin allowed the change of sign for initial vortex sheet, but assumed special reflection symmetry to prove existence of global weak solutions. Related to this problem is the one of characterizing the precise borderline function space to which initial data belongs, and above which there is no concentration phenomenon for weakly approximating sequence of solutions; a recent analysis of this problem was done by E Tadmor in 2001.

For the uniqueness problem of the weak solutions of the 2D Euler equations, there are remarkable works by V Scheffer (1993) and A Shnirelman (1997), where they constructed explicitly an $L^2_{\mathrm{loc}}(\mathbb{R}^2 \times \mathbb{R})$ weak solution starting from zero initial data. Also M Vishik (1999) extended the uniqueness class of the weak solutions of the 2D Euler equations, improving previous work by V Yudovich (1995). The class found by M Vishik, in particular, includes the BMO. There is another problem closely related to the weak solutions of the 2D Euler equations, called the vortex patch problem. The main question was if there is any singularity of the boundary of a patch $\Omega(t) = \{X(\alpha,t) \mid \alpha \in \Omega_0\}$, where $X(\alpha,t)$ is the particle trajectory mapping generated by a weak solution $v(x,t)$, which is evolving from the initial data $\omega_0(x) = \chi_{\Omega_0}(x)$, the characteristic function of set Ω_0

with smooth boundary. The problem itself is well defined, due to the work of V Yudovich (1963), and there exists unique particle trajectories associated with such weak solutions. The problem was settled by J-Y Chemin in 1991. He proved the global-in-time preservation of the $C^{1,\alpha}$ regularity of the boundary $\partial\Omega(t)$, contrary to the previous numerical experiments. The proof of this result was later simplified by A Bertozzi and P Constantin in 1993.

Another interesting problem related to the weak solutions of the Euler equations (2D or 3D) is whether or not the energy is preserved for the weak solutions, namely if there is any "intrinsic dissipation" to the singular solutions of the ideal fluids. In 1949, L Onsager conjectured that if the weak solution of 3D Euler equations belongs to certain Hölder space, then the energy is conserved. This conjecture, in the setting of Besov space, was proved by P Constantin, W E and E S Titi in 1994. This question of possibility of dissipation of energy for weak solutions is further studied by J Duchon and R Robert in 2000. Later, in 2003 the present author considered the problem of helicity conservation for the weak solutions of the 3D Euler flows, which is related to the question of crossing/reconnections of the vortex tubes for weak solutions, and showed that for large class of weak solutions in certain Besov spaces the helicity is preserved.

See also: Compressible Flows: Mathematical Theory; Evolution Equations: Linear and Nonlinear; Fluid Mechanics: Numerical Methods; Interfaces and Multicomponent Fluids; Intermittency in Turbulence; Inviscid Flows; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Stability of Flows; Stochastic Hydrodynamics; Turbulence Theories; Viscous Incompressible Fluids: Mathematical Theory; Vortex Dynamics.

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Indefinite Metric

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Introduction

If, in a problem of quantization, state spaces with indefinite inner product are used instead of Hilbert spaces, one speaks of quantization with indefinite metric. The main domain of application is the quantization of gauge fields, like the electromagnetic vector potential $A_\mu(x)$ or Yang–Mills fields in quantum chromodynamics (QCD) and the standard model.

The conceptual problem with the indefinite metric is the occurrence of senseless negative probabilities in the formalism. Such negative probabilities, however, only arise in expectation values of fields that are not gauge invariant and hence do not correspond to observable quantities. Equivalently, the inner product of vectors generated by application of such fields to the vacuum vector with itself can be negative or null. In order to extract the observable content of an indefinite-metric quantum theory, a subsidiary condition is needed to single out the physical subspace. Restricted to this subspace, the inner product is positive semidefinite. This subsidiary condition can be seen as the implementation of a gauge, as, for example, the Lorentz gauge $\partial_\mu A^\mu(x) = 0$ in quantum electrodynamics (QED). This procedure is also known under the name Gupta–Bleuler formalism.

The use of indefinite metric in the quantization of gauge theories like QED can be avoided entirely.

This is called quantization in a physical gauge. The problem with such gauges is that they are not Lorentz invariant and that the vector potential $A^{\mu}(x)$ is not a local field. An example is the Coulomb gauge defined by $A_0(x) = 0$ and $\partial^i A_i(x) = 0$ in QED. Furthermore, Dirac spinor fields $\psi(x)$ in such gauges do not anticommute when localized in spacelike separated regions. The Dirac fields therefore are also nonlocal quantities. Although not in contrast with special relativity, as Dirac spinors and the vector potential are not gauge invariant and hence are unobservable, this leads to severe technical problems in the formulation of interacting theories. In particular, the theory of renormalization heavily uses both locality and invariance. Therefore, the Gupta–Bleuler formalism generally is the preferred quantization procedure for a gauge theory.

That a local and invariant quantization is not possible using a (positive-metric) Hilbert space has been proved by F Strocchi in a series of articles published between 1967 and 1970. If one wants to preserve locality and/or invariance of the quantized field theory, it is thus strictly necessary to give up the positivity of the state space.

A short digression into the early history of the idea might be of interest. It dates back to 1941, where the use of indefinite metric in the quantization of relativistic equations was proposed by Paul Dirac in a lecture at the London Royal Society. The negative probabilities for the bosonic vector potential were thought to be connected with the problem of negative-energy solutions of relativistic equations as a type of surrogate of the "Dirac sea" in the quantization of fermions. Furthermore, Dirac proposed that negative-energy solutions and negative probabilities would jointly lead to the cancellation of divergences in QED. The latter idea was taken up by W Heisenberg in his lectures on the theory of elementary particles held in Munich in 1961, but the generally accepted solution to the problem of ultraviolet divergences was achieved without recourse to Dirac's original motivation. In 1950 the consistent quantization of vector potential in the Lorentz gauge was formulated by SN Gupta and K Bleuler eliminating the use of negative-energy solutions. Since then the indefinite metric has become a building block of the standard theory of quantized gauge fields.

No-Go Theorems

The strict necessity of the Gupta–Bleuler procedure for the local or covariant quantization of gauge fields has been demonstrated by F Strocchi in the form of no-go theorems for positive metric. Here we review their content for the case of the electromagnetic field. Related statements can be obtained for nonabelian gauge theories. The main problem lies in the fact that standard assumptions on the quantization of relativistic fields are in conflict with Maxwell equations that should hold as operator identities in a positive-metric theory containing no unobservable states. Let

$$F_{\nu\mu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) \qquad [1]$$

be the quantized electromagnetic field strength tensor. Classically, the existence of $A_\mu(x)$ is guaranteed from the first set of Maxwell equations $\epsilon^{\alpha\beta\nu\mu}\partial_\beta F_{\nu\mu}(x) = 0$. Here (and henceforth) indices are raised and lowered with respect to the Minkowski metric $g_{\alpha\beta}$ and $\epsilon^{\alpha\beta\mu\nu}$ is the completely antisymmetric tensor on $\mathbb{R}^d$. Furthermore, we apply Einstein's convention on summation over repeated upper and lower indices. Standard assumptions from axiomatic quantum field theory are:

1. The field strength tensor $F_{\nu\mu}(x)$ is an operator-valued distribution acting on a (dense core of a) Hilbert space $\mathcal{H}$ with scalar product $\langle .,. \rangle$ – in the indefinite-metric case, $\langle .,. \rangle$ only needs to be an inner product.
2. $F_{\mu\nu}(x)$ transforms covariantly, that is, there is a strongly continuous unitary (with respect to $\langle .,. \rangle$) representation U of the orthochronous, proper Poincaré group on $\mathcal{H}$ such that for translation $a \in \mathbb{R}^d$ combined with a restricted Lorentz transformation Λ, one has
$$U(a,\Lambda)F_{\mu\nu}(x)U(a,\Lambda)^{-1} = (\Lambda^{-1})^{\rho}{}_{\mu}(\Lambda^{-1})^{\kappa}{}_{\nu}F_{\rho\kappa}(\Lambda x + a) \qquad [2]$$
3. There exists a unique (up to multiplication with $\mathbb{C}$-numbers) translation invariant vector $\Omega \in \mathcal{H}$ (the "vacuum"), that is, $U(a,1)\Omega = \Omega \forall a \in \mathbb{R}^d$.
4. The representation of the translations fulfills the spectral condition
$$\int_{\mathbb{R}^4} \langle \Phi, U(a,1)\Psi \rangle e^{ip\cdot a}\, da = 0 \qquad [3]$$
$\forall \Psi, \Phi \in \mathcal{H}$ if p is not in the closed forward light cone $\bar{V}^+ = \{p \in \mathbb{R}^4 : p \cdot p \geq 0, p^0 \geq 0\}$. Here the dot is the Minkowski inner product.
So far the assumptions concerned only observable quantities. In the following, we also demand.
5. The vector potential $A_\mu(x)$ is realized as an operator-valued distribution on $\mathcal{H}$ and transforms covariantly under translations
$$U(a,1)A_\mu(x)U(a,1)^{-1} = A_\mu(x+a) \qquad [4]$$

The assumptions on the nature of the vector potential so far are rather weak. Strocchi's no-go theorems show that one cannot add further desirable properties as Lorentz covariance and/or locality without getting into conflict with the Maxwell equations:

Theorem 1 *Suppose that the above assumptions* (1)–(3) *and* (5) *hold. If Maxwell's equations in the absence of charges,*

$$\epsilon^{\alpha\beta\nu\mu}\partial_\beta F_{\nu\mu}(x) = 0, \quad \partial^\mu F_{\mu\nu}(x) = 0 \qquad [5]$$

are valid as δ operator identities on $\mathcal{H}$ and the gauge potential transforms covariantly

$$U(a,\Lambda)A_\mu(x)U(a,\Lambda)^{-1} = (\Lambda^{-1})^\nu{}_\mu A_\nu(\Lambda x + a) \qquad [6]$$

the two-point function of the electromagnetic field tensor vanishes identically:

$$\langle \Omega, F_{\nu\mu}(x)F_{\kappa\rho}(y)\Omega\rangle = 0 \quad \forall\, x,y \in \mathbb{R}^4 \qquad [7]$$

To gain a better understanding, where the difficulties in the quantization of the Maxwell equations arise from, here is a rough sketch of the proof: Maxwell equations and covariance imply that $f_{\mu\nu\rho}(x-y) = \langle \Omega, A_\mu(x)F_{\nu\rho}(y)\Omega\rangle$ fulfills $\partial^\alpha\partial_\alpha f_{\mu\nu\rho}(x) = 0$ and hence its Fourier transform has support in the union of the forward and backward light cone. The Fourier transform thus can be split into a positive- and a negative-frequency part, and $f_{\mu\nu\rho} = f^+_{\mu\nu\rho} + f^-_{\nu\mu\rho}$ accordingly. By the general analysis of axiomatic field theory (*see* Axiomatic Quantum Field Theory), the functions $f^\pm_{\nu\mu\rho}$ are boundary values of complex analytic functions on certain tubar domains $\mathcal{T}^\pm$ transforming covariantly under a certain representation of the complex Lorentz group. By a theorem of Araki and Hepp giving a general representation of such functions and using the antisymmetry of the field tensor, the following formula can be derived:

$$f^\pm_{\mu\nu\rho}(z) = (g_{\mu\rho}\partial_\nu - g_{\mu\nu}\partial_\rho)f^\pm(z) + \epsilon_{\mu\nu\rho\alpha}\partial^\alpha h^\pm(z)$$
$$z \in \mathcal{T}^\pm \qquad [8]$$

with $f^\pm, h^\pm$ invariant under complex Lorentz transformations. Taking boundary values in $\mathcal{T}^\pm$, one obtains $f_{\mu\nu\rho} = (g_{\mu\rho}\partial_\nu - g_{\mu\nu}\partial_\rho)f + \epsilon_{\mu\nu\rho\alpha}\partial^\alpha h$, with $f = \bar{f}^+ + \bar{f}^-$ and $h = \bar{h}^+ + \bar{h}^-$, where the bar stands for the distributional boundary value. Maxwell's equations imply $\partial^\nu f_{\mu\nu\rho} = (\partial^\nu\partial_\nu g_{\mu\rho} - \partial_\mu\partial_\rho)f = 0$ and $\epsilon_\alpha{}^{\beta\nu\rho}\partial_\beta f_{\mu\nu\rho} = (\partial^\nu\partial_\nu g_{\alpha\mu} - \partial_\alpha\partial_\mu)h = 0$. The only Lorentz-invariant solutions to these equations are constant, which implies the statement of Theorem 1.

The second no-go theorem eliminates the assumption that the vector potential $A_\mu(x)$ is covariant; however, a local gauge is assumed. The result is the same as in Theorem 1:

Theorem 2 *Suppose that the above assumptions* (1)–(5) *and Maxwell's equations hold as operator identities on $\mathcal{H}$. If, furthermore, the gauge is local, that is,*

$$[A_\mu(x), A_\nu(y)] = 0 \quad \text{if } x-y \text{ is spacelike} \qquad [9]$$

the two-point function of the field strength tensor vanishes again as in Theorem 1.

Analyzing the interplay of the covariance properties of $F_{\mu\nu}(x)$ with the locality of $A_\mu(x)$, Strocchi was able to show that the function $f_{\mu\nu\rho}(x-y)$ must have the same covariance properties as in Theorem 1, which implies the assertion of Theorem 2.

The first two no-go theorems deal with the free electromagnetic field that is not coupled to charge-carrying fields. This is, of course, already a real obstruction also for an interacting theory, since, by the LSZ formalism, one expects the asymptotic incoming and outgoing fields $A^{\text{in/out}}_\mu(x), F^{\text{in/out}}_{\mu\nu}(x)$ to be free. In fact, it has been proved by D Buchholz that, in the positive-metric case, such asymptotic fields can always be constructed. If one assumes a local and covariant gauge and positivity, the vanishing of the two-point function would also imply that the field $F_{\mu\nu}(x) = 0$ identically by the Reeh–Schlieder theorem.

The next no-go theorem shows that the problems connected to the quantization of the Maxwell equations are not connected only to the free electromagnetic fields. Let us assume that the second set of Maxwell equations is given by

$$\partial^\mu F_{\mu\nu}(x) = j_\nu(x) \qquad [10]$$

where j_ν is the leptonic current, that is, $j_\nu(x) = e : \psi^\dagger(x)\gamma_\nu\psi(x):$ in the case of QED, where ψ is the quantized Dirac field associated with electrons and positrons. Here $: \cdot :$ stands for Wick ordering and γ_ν are the Dirac matrices, $\psi^\dagger = \psi^*\gamma^0$. The conservation of the current $\partial^\nu j_\nu(x) = 0$ implies that the current charge

$$Q_C = \lim_{R\to\infty}\int_{\mathbb{R}^3}\int_{\mathbb{R}} \alpha(x^0)\chi(\boldsymbol{x}/R)j_0(x^0,\boldsymbol{x})\,dx^0\,d\boldsymbol{x} \qquad [11]$$

is a constant of motion, where α and χ are compactly supported infinitely differentiable functions with $\int_{\mathbb{R}}\alpha(x^0) = 1$ and $\chi(\boldsymbol{x}) = 1$ for $|\boldsymbol{x}| < 1$. Now, an alternative definition of charge, called gauge charge (it generates the global U(1)-gauge transformation), is given by

$$Q_G\Omega = 0, \quad [Q_C, A_\mu(x)] = 0 \quad \text{and}$$
$$[Q_G, \psi(x)] = -e\psi(x) \qquad [12]$$

A third formulation of charge, the Maxwell charge Q_M, can also be given by replacing $j^0(x)$ in [11] by $\partial_\nu F^{\nu 0}(x)$. Obviously, if Maxwell equations hold as operator identities, $Q_C = Q_M$. On observable states, all charges Q_M, Q_C, and Q_G ought to coincide. Strocchi's third theorem shows that this cannot be achieved within a local gauge:

Theorem 3 *If the Maxwell equations* [9] *hold and the Dirac field* $\psi(x)$ *is local with respect to the electromagnetic field tensor* $F_{\mu\nu}(x)$, *that is,*

$$[F_{\mu\nu}(x), \psi(y)] = 0 \quad \text{if } x - y \text{ is spacelike} \qquad [13]$$

then $[Q_M, \psi(x)] = 0$, *hence* $Q_C = Q_M \neq Q_C$.

The proof is a simple consequence of the observation that $j_0(x) = \partial^\nu F_{\nu 0}(x) = \partial^i F_{i0}(x)$ is a three-divergence as $F_{00}(x) = 0$ by antisymmetry of $F_{\mu\nu}(x)$. Hence,

$$\begin{aligned}[Q_C, \psi(y)] &= \lim_{R\to\infty} \int_{\mathbb{R}^4} [j_0(x), \psi(y)] \alpha(x^0) \chi(\mathbf{x}/R)\, dx^0\, d\mathbf{x} \\ &= -\lim_{R\to\infty} \int_{\mathbb{R}^4} [F_{i0}(x), \psi(y)] \alpha(x^0) \partial^i \chi(\mathbf{x}/R) \\ &\quad \times dx^0\, d\mathbf{x} = 0 \end{aligned} \qquad [14]$$

since, for R sufficiently large, the support of $\alpha(x^0)\partial_i \chi(\mathbf{x}/R)$ becomes spacelike separated from y.

It should be noted that the proof of none of the above theorems relies on the definiteness of the inner product. The main clue of the indefinite-metric formalism, therefore, is rather to give up Maxwell equations as operator identities. In the usual positive-metric formalism, where all states in $\mathcal{H}$ are physical states, this would not be legitimate. But in indefinite metrics, many states are unobservable – in particular, those with negative "norm" $\langle \Psi, \Psi \rangle < 0$. On such states we can neglect the Maxwell equations.

Axiomatic Framework

The formalism of axiomatic quantum field theory (*see* Axiomatic Quantum Field Theory) requires a revision in order to cover the case of gauge fields. The necessary adaptations have been elaborated by G Morchio and F Strocchi, but also earlier work of E Scheibe and J Yngvasson played a significant role in this development.

Let $\phi(x)$ be a V'-valued quantum field, where V is a finite-dimensional $\mathbb{C}$-vector space with involution $*$. The prime stands for the (topological) dual. For the case of QED, V is eight dimensional, containing four dimensions for the vector potential $A_\mu(x)$ and another four for the Dirac spinors $\psi(x), \psi^\dagger(x)$.

Such a quantum field can be reconstructed from its vacuum expectation values (Wightman functions) as follows: let $S_1 = S(\mathbb{R}^4, V)$ be the space of rapidly decreasing functions $f: \mathbb{R}^4 \to V$ endowed with the Schwarz topology. Then the Borcher's algebra $\underline{S}$ be the free, unital, involutive tensor algebra over $\mathcal{S}_1$, that is, $\underline{S} = \mathbb{C}\mathbf{1} \oplus_{n\geq 0} \mathcal{S}_1^{\otimes n}$ with the multiplication induced by the tensor product and involution $(f_1 \otimes \cdots \otimes f_n)^* = f_n^* \otimes \cdots \otimes f_1^*$. $\underline{S}$ is endowed with the direct-sum topology. One can show that any linear, normalized, continuous functional $\underline{W}: \underline{\mathcal{S}} \to \mathbb{C}, W(\mathbf{1}) = 1$, is determined by its restrictions W_n to $\mathcal{S}_1^{\otimes n}$. By the Schwarz kernel theorem, $W_n \in \mathcal{S}'(\mathbb{R}^{4n}, V^{\otimes n})$. Conversely, any such sequence of Wightman distributions W_n determines a $\underline{W}$.

Given a Hermitian Wightman functional $\underline{W}$ such that $W(f^*) = \overline{W(f)}, \forall f \in \underline{S}, \mathcal{L}_{\underline{W}} = \{f \in \underline{S}: \underline{W}(h^* \otimes f) = 0\, \forall \underline{h} \in \underline{S}\}$ forms a left ideal and the inner product $\underline{W}(f^* \otimes \underline{h})$ induces a nondegenerate inner product $\langle .,. \rangle$ on $\mathcal{H}_0 = \underline{S}/\mathcal{L}_{\underline{W}}$. Furthermore, Borchers' algebra $\underline{S}$ acts from the left on $\mathcal{H}_0$. The quantum field $\phi(x)$ defined as the restriction of this canonical representation to the space $\mathcal{S}_1 \subset \underline{S}$ according to $\phi(f) =$ "$\int_{\mathbb{R}^4} \phi^a(x) f_a(x) dx$" where the index a runs over a basis of V.

If the Wightman functional $\underline{W}$ has further properties from axiomatic QFT (*see* Axiomatic Quantum Field Theory) like invariance with respect to a given representation of the Lorentz group on V, translation invariance, locality, and the spectral property, the quantum field $\phi(x)$ fulfills the related requirements in analogy with the items (1)–(5) listed in the previous section for the case of the vector potential $A_\mu(x)$. The Wightman distributions W_n as in the positive-metric case are related to the vacuum expectation values of the theory by

$$W_n^{a_1,\ldots,a_n}(x_1,\ldots,x_n) = \langle \Omega, \phi^{a_1}(x_1) \cdots \phi^{a_n}(x_n) \Omega \rangle \qquad [15]$$

where Ω is the equivalence class of $\mathbf{1}$ in $\mathcal{H}_0$.

The state-space $\mathcal{H}_0$ produced by the Gelfand–Naimark–Segal (GNS) construction for inner-product spaces might be too small to contain all states of physical interest. For example, in the QED case, it does not contain charged states (cf. Theorem 3). Depending on the physical problem, one might also be interested in constructing coherent or scattering states and translation-invariant states apart from the vacuum. Such states appear in problems related to symmetry breaking and confinement (the so-called Θ-vacua) or in some problems of conformal QFT (*see* Boundary Conformal Field

Theory) in two dimensions. It, therefore, has become the standard point of view that one needs to make a suitable closure of $\mathcal{H}_0$ such that this closure includes the states of interest (for an alternative point of view, see the last paragraph of the following section).

Typically, larger closures are favorable, as they contain more states. One therefore focuses on maximal Hilbert closures of $\mathcal{H}_0$. A Hilbert topology τ is induced by an auxiliary scalar product $(.,.)$ on $\mathcal{H}_0$. It is admissible, if it dominates the indefinite inner product $|\langle\Phi,\Psi\rangle|^2 \leq C(\Psi,\Psi)(\Phi,\Phi)\,\forall\Psi,\Phi\in\mathcal{H}_0$ for some $C>0$. This guarantees that the inner product extends to the Hilbert space closure $\mathcal{H}$ of $\mathcal{H}_0$ with respect to τ. Furthermore, there exists a self-adjoint contraction η on $\mathcal{H}$ such that $\langle\Psi,\eta\Phi\rangle = (\Psi,\eta\Phi)\,\forall\Phi,\Psi\in\mathcal{H}$. A Hilbert topology τ is maximal if there is no admissible Hilbert topology τ' that is strictly weaker than $\mathcal{H}_0$. The classification of maximal admissible Hilbert topologies in terms of the metric operator η is given by the following theorem:

Theorem 4 *A Hilbert topology τ on $\mathcal{H}_0$ generated by a scalar product $(.,.)$ is maximal if and only if the metric operator η has a continuous inverse η^{-1} on the Hilbert space closure $\mathcal{H}$ of $\mathcal{H}_0$. In that case, one can replace $(.,)$ by the scalar product $(\Psi,\Phi)_1 = (\Psi,|\eta|\Phi)$ without changing the topology τ. The new metric operator η_1 then fulfills $\eta_1^2 = 1_{\mathcal{H}}$.*

For a proof of the first statement, see the original work of Morchio and Strocchi (1980). One can easily check that $\eta_1 = \eta|\eta^{-1}|$ which implies the second assertion of the theorem. A Hilbert space $(\mathcal{H},(.,.))$ with an indefinite inner product induced by a metric operator η with $\eta^2 = 1_{\mathcal{H}}$ is called a Krein space. For an extensive study of Krein spaces, see the monograph by Azizov and Iokhvidov (1989).

Furthermore, one can show that given a nonmaximal admissible Hilbert space topology τ induced by some $(.,.)$, one obtains a maximal admissible Hilbert topology as follows: given the metric operator η, we define a scalar product $(\Psi,\Phi)_1 = (\Psi,(1-P_0)\Phi)$ on $\mathcal{H}$ with P_0 the null space projector of η. Obviously, this scalar product is still admissible and it leads to a new metric operator η_1 and a new closure $\mathcal{H}_1$ of $\mathcal{H}_0$. Furthermore, it is easy to show that the scalar product $(\Psi,\Phi)_2 = (\Psi,|\eta_1|\Phi)_1$ still induces an admissible Hilbert topology which is also maximal, as $\eta_2 = \eta_1|\eta_1^{-1}|$ clearly fulfills the Krein relation $\eta_2^2 = 1_{\mathcal{H}_2}$.

The question of the existence of a Krein space closure of $\mathcal{H}_0$, therefore, reduces to the question of the existence of an admissible Hilbert topology on $\mathcal{H}_0$. The following condition on the Wightman functions W_n replaces the positivity axiom in the case of indefinite-metric quantum fields:

Theorem 5 *Given a Wightman functional $\underline{W}$, there exists an admissible Hilbert space topology τ on $\mathcal{H}_0 = \underline{S}/\mathcal{L}_{\underline{W}}$ if and only if there exists a family of Hilbert seminorms p_n on $\mathcal{S}_n$ such that $|W_{n+n}(f\otimes h)| \leq p_n(f)p_m(h), \forall n, m\in\mathbb{N}_0, f\in\mathcal{S}_n, h\in\mathcal{S}_m$.*

In some cases, covering also examples with nontrivial scattering in arbitrary dimension, the condition of Theorem 5 can be checked explicitly (*see* Non-trivial Models of Quantum Fields with Indefinite Metric).

It should be mentioned that different choices of the Hilbert seminorms p_n lead to potentially different maximal Hilbert space closures (Hoffmann 1998, Constantinescu and Gheondea 2001). In fact, often the topology is not even Poincaré invariant and hence the states that can be approximated with local states depend on a chosen inertial frame. This fact, for the case of QED, has been interpreted in terms of physical gauges.

Many results from axiomatic field theory (*see* Axiomatic Quantum Field Theory) with positive metric also hold in the case of QFT with indefinite metric, like the PCT and the Reeh–Schlieder theorem, the irreducibility of the field algebra (for massive theories) and the Bisoniano–Wichmann theorem (*see* Algebraic Approach to Quantum Field Theory). Other classical results, like the Haag–Ruelle scattering theory and the spin and statistics theorem definitively do not hold, as has been proved by counterexamples. This is, however, far from being a disadvantage, as, for example, it permits the introduction of various gauges in the scattering theory of the vector potential $A_\mu(x)$ and fermionic scalar "ghost" fields in the BRST quantization (*see* BRST Quantization) formalism.

Gupta–Bleuler Gauge Procedure

Here the Gupta–Bleuler gauge procedure is presented in a slightly generalized form following Steinmann's monograph. Classically, the equations of motion for the vector potential $A_\mu(x)$,

$$\partial^\nu\partial_\nu A_\mu(x) + \lambda\partial_\mu\partial^\nu A_\nu(x) = j_\mu(x) \qquad [16]$$

together with Lorentz gauge condition $B(x) = \partial_\mu A^\mu(x) = 0$ imply the Maxwell equations [10]. Here, $\lambda\in\mathbb{R}$ plays the role of a gauge parameter. As seen above, both equations, the so-called pseudo-Maxwell equations [16] and the Lorentz gauge condition $B(x) = 0$, cannot both hold as operator identities. The idea for the quantization

of the theory therefore is to give up the Lorentz gauge condition as an operator identity on the entire state space $\mathcal{H}$.

Suppose one has constructed such a theory with an indefinite inner state space $\mathcal{H}$. Already for the noninteracting theory, any invariant, spectral, local, and covariant solution requires indefinite metric, cf. the explicit formula [18] below. To complete the Gupta–Bleuler program, one needs to find a subspace of (equivalence classes of) physical states $\mathcal{H}'$ of the inner-product space $\mathcal{H}'$ such that the following conditions hold:

1. the vacuum is a physical state, that is, $\Omega \in \mathcal{H}'$;
2. observable fields like $j_\mu(x)$ and $F_{\nu\mu}(x)$ map $\mathcal{H}'$ to itself;
3. the inner product $\langle .,. \rangle$ restricted to $\mathcal{H}'$ is positive semidefinite;
4. observable fields map $\mathcal{H}''$, the set of null vectors in $\mathcal{H}'$, to itself; and
5. the Maxwell equations hold on $\mathcal{H}'$ in the sense

$$\langle \Psi, \partial^\nu F_{\nu\mu}(x)\Phi \rangle = \langle \Psi, j_\mu(x)\Phi \rangle, \quad \forall \Psi, \Phi \in \mathcal{H}' \qquad [17]$$

Then one obtains $\mathcal{H}^{\mathrm{ph}}$ as the completion of the quotient space $\mathcal{H}'/\mathcal{H}''$. The physical Hilbert space $\mathcal{H}^{\mathrm{ph}}$ contains the vacuum Ω (1), observable fields act on $\mathcal{H}^{\mathrm{ph}}$ (2) and (4), it is a Hilbert space (3) and the Maxwell equations hold on it (5).

To see that such a construction is possible, consider the noninteracting case $j_\nu(x) = 0$, that is, the limit case of vanishing electrical charge $e \to 0$, first. By taking the divergence of [16], one obtains $(1-\lambda)\partial^\nu \partial_\nu \partial^\mu A_\mu(x) = 0$. Excluding the Landau gauge ($\lambda = 1$), this implies $(\partial^\nu \partial_\nu)^2 A_\mu(x) = 0$. The most general solution for the two-point vacuum expectation values that is in agreement with [16] and the requirements of locality, translation invariance, the spectral condition, uniqueness of the vacuum, and the Lorentz covariance of $A^\mu(x)$ is then

$$\begin{aligned} &\langle \Omega, A_\nu(x) A_\mu(y) \Omega \rangle \\ &\quad = (-g_{\mu\nu} + \rho \partial_\mu \partial_\nu) D^+(x-y) \\ &\qquad + \frac{\lambda}{1-\lambda} \partial_\mu \partial_\nu E^+(x-y) \end{aligned} \qquad [18]$$

where D^+ and E^+ are the inverse Fourier transforms of $\theta(p^0)\delta(p^2)$ and $\theta(p^0)\delta'(p^2)$ respectively, $p^2 = p \cdot p$, θ being the Heavyside function, δ the Dirac measure on $\mathbb{R}$ of mass one in zero and δ' its derivative. ρ and λ are gauge parameters, for example, the Feynman gauge corresponds to $\lambda = \rho = 0$. We have also omitted an overall factor corresponding to a field strength normalization (choice of numerical value of $\hbar$ – here $\hbar = 1$).

Using Wick's theorem and the GNS construction for inner-product spaces (cf. the preceding section), it is possible to realize a representation of the vector potential $A_\nu(x)$ as operator-valued distribution on some indefinite-metric state space $\mathcal{H}$ with Fock structure, for example, a Krein closure of the GNS space with Ω the GNS vacuum and $\mathcal{D} \subseteq \mathcal{H}$ the canonical domain of definition. In the case of Feynman gauge, the metric operator η can be obtained by a second quantization of the operator $f_\mu \to \sum_{\nu=1}^{4} g_{\mu\nu} f_\nu$ on the one-particle space $\mathcal{S}_1$.

In particular, the field $B(x)$ acts as an operator-valued distribution on $\mathcal{H}$ and, by taking the divergence of [16], it follows that $\partial^\nu \partial_\nu B(x) = 0$. Thus, $B(x) = B^+(x) + B^-(x)$ can be decomposed into a positive ("annihilation") and a negative ("creation") frequency part $B^\pm(x)$. One obtains:

Theorem 6 *The space* $\mathcal{H}' = \{\Psi \in \mathcal{D}: B^+(x)\Psi = 0\}$ *fulfills all requirements* (1)–(5) *of the Gupta–Bleuler gauge procedure.*

Condition (1) is obvious and (2) follows from the fact that the fields $F_{\nu\mu}(x)$ and $B(x)$ commute, which can be checked on the level of two-point functions [18]. In the same spirit, one can also use [18] to check (3) and (4) by explicit calculations on the one-particle space and showing that $\mathcal{H}'$ is the Fock space over the one-particle states annihilated by $B^+(x)$. Finally, by Hermiticity of $A^\mu(x), B^+(x)^* = B^-(x)$ and thus $\langle \Psi, B(x)\Phi \rangle = \langle \Psi, B^+(x)\Phi \rangle + \langle B^+(x)\Psi, \Phi \rangle = 0$. As the field $B(x)$ stands for the obstruction to Maxwell equations, this implies condition (5).

It should be noted that the physical state space $\mathcal{H}^{\mathrm{ph}}$ does not depend on the gauge parameters λ, ρ and that it is spanned by repeated application of the field tensor $F_{\mu\nu}(x)$ to the vacuum.

By current conservation, the divergence of [16] still yields $\partial^\nu \partial_\nu B(x) = 0$ also in the interacting case where $e \neq 0$. One can then choose the same gauge condition as in Theorem 6 to define $\mathcal{H}'$. One can then try to prove that this space fulfills all the requirements of the Gupta–Bleuler procedure, for example, in the sense of perturbation theory. Using more advanced formulations as, for example, BRST quantization and Bogoliubov's local S-matrix formalism, this program has been completed up to a solution of the infrared problem (*see* Perturbative Renormalization Theory and BRST).

A different procedure, motivated by the necessity of coincidence of all charges Q_C, Q_G, and Q_M on the physical state space, has been elaborated by Steinmann. It deviates from the standard procedure in the sense that the physical space $\mathcal{H}'$ is not included in $\mathcal{H}$, but $\mathcal{H}^{\mathrm{ph}}$ is directly obtained from the GNS procedure after taking certain limits of Wightman functions restricted to

certain gauge-invariant algebras constructed from the Borchers algebra and a limiting procedure in a gauge parameter. The Wightman functional on this gauge-invariant algebras are positive (in the sense of perturbation theory), the limiting procedure, however, implies that the so-obtained physical states are singular (i.e., have diverging inner product) to states in $\mathcal{H}$, hence the so-defined state spaces corresponding to going to a physical gauge after solving the problem of a perturbative construction of an indefinite-metric solution, are not subspaces of $\mathcal{H}$.

See also: Algebraic Approach to Quantum Field Theory; Axiomatic Approach to Topological Quantum Field Theory; Axiomatic Quantum Field Theory; Boundary Conformal Field Theory; BRST Quantization; Perturbative Renormalization Theory and BRST; Quantum Fields with Indefinite Metric: Non-Trivial Models.

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Index Theorems

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Introduction

Let g be a Riemannian metric on a smooth compact manifold M of dimension m. We assume for the moment that the boundary of M is empty and postpone until later a discussion of the more general setting. If $x=(x_1,\ldots,x_m)$ is a local system of coordinates on M, let

$$g_{ij} := g\left(\partial_i^x, \partial_j^x\right)$$

give the components of the metric tensor. Let D be an operator of Laplace type on a smooth vector bundle V over M. Adopt the Einstein convention and sum over repeated indices. Relative to a local coordinate frame for V, D has the form

$$D = -\left\{g^{ij}\mathrm{Id}\partial_i^x\partial_j^x + A^k\partial_k^x + B\right\}$$

where A^k and B are endomorphisms (i.e., matrices) of V.

We assume that V is equipped with a positive-definite inner product and that D is self-adjoint. There is then a complete orthonormal basis $\{\phi_i\}$ for $L^2(V)$, where $\phi_i \in C^\infty(V)$ and $D\phi_i = \lambda_i\phi_i$. The collection $\{\phi_i, \lambda_i\}$ is called a discrete spectral resolution of D. For example, if $D = -\partial_\theta^2$ on the circle, then the discrete spectral resolution is

$$\left\{e^{\sqrt{-1}n\theta}, n^2\right\}_{n\in\mathbb{Z}}$$

If we order the eigenvalues $\lambda_1 \le \lambda_2 \le \cdots$ and repeat each eigenvalue according to multiplicity, then there is the following estimate due to Weyl:

$$\lambda_n \sim n^{2/m} \quad \text{as} \quad n \to \infty$$

We now suppose given a pair of vector bundles V_1 and V_2 over M and a kth-order partial differential elliptic operator

$$A : C^\infty(V_1) \to C^\infty(V_2)$$

Locally, we decompose

$$A = \sum_{|I| \le k} a_I \partial_x^I$$

where $I = (i_1, \ldots, i_m)$ is a multi-index and where

$$\partial_x^I = (\partial_1^x)^{i_1} \ldots (\partial_m^x)^{i_m}$$

The a_I are linear maps from V_1 to V_2. The leading symbol of A is then defined by setting

$$\sigma_L(A)(x, \xi) := (\sqrt{-1})^k \sum_{|I|=k} a_I(x) \xi^I$$

where $\xi^I = (\xi_1)^{i_1} \ldots (\xi_m)^{i_m}$, and

$$\xi = (\xi_1, \ldots, \xi_m)$$

are local fiber coordinates on the cotangent bundle. The leading symbol is an invariantly defined map

$$\sigma_L : T^*M \to \mathrm{End}(V_1, V_2)$$

For example, if $V_1 = V_2$ and if D is an operator of Laplace type, then the leading symbol is given by the metric tensor, that is,

$$\sigma_L(D) = g^{ij} \xi_i \xi_j \mathrm{Id} = |\xi|^2 \mathrm{Id}$$

If d is exterior differentiation, then the leading symbol is given by exterior multiplication, that is,

$$\sigma_L(d)(\xi)\omega = \sqrt{-1}\xi \wedge \omega$$

The operator A is said to be elliptic if $\sigma_L(A)$ is an isomorphism from V_1 to V_2 for any $\xi \ne 0$. If A is an elliptic partial differential operator, then

$$\begin{aligned} \mathrm{index}(A) &:= \dim \ker(A) - \dim \mathrm{coker}(A) \\ &= \dim \ker(A^*A) - \dim \ker(AA^*) \end{aligned}$$

is well defined. As the index vanishes if m is odd, we assume for the most part that m is even.

If A_ε is a smooth one-parameter family of such operators, then index (A_ε) is independent of ε. The index depends only on the homotopy class of the leading symbol of A within the class of invertible symbols; it does not depend on the underlying metric of the manifold and it does not depend on the fiber metrics chosen for V_1 and V_2.

The Atiyah–Singer index theorem expresses the index as the integral of suitably chosen polynomials in the curvature tensor for the classical elliptic complexes and, more generally, in terms of cohomological information for general elliptic complexes. Further details appear later in the article.

The primary focus here is on the complexes which are of Dirac type, that is, complexes where A is a first-order partial differential operator and where the associated second operators $D_1 := A^*A$ and $D_2 := AA^*$ are of Laplace type.

Here is a brief outline of this article. The classical elliptic complexes (de Rham, signature, spin, Dolbeault, Yang–Mills) are discussed first. Next the characteristic classes are introduced, followed by the relevant formula for the index of the classical elliptic complexes, manifolds with boundary, and the equivariant index. Index theory is an enormous topic and here only classical features are emphasized as a complete treatment is beyond the scope of a short expository note such as this one. As some guide to various applications in mathematical physics, the reader is referred to the Further Reading section.

The Classical Elliptic Complexes

The de Rham Complex

Let $\Lambda^p M$ be the bundle of smooth p forms over M and let

$$d : C^\infty(\Lambda^p M) \to C^\infty(\Lambda^{p+1} M)$$

and

$$\delta : C^\infty(\Lambda^p M) \to C^\infty(\Lambda^{p-1} M)$$

be the exterior derivative and dually the interior derivative, respectively. We set

$$\Delta := (d + \delta)^2 \quad \text{on} \quad C^\infty(\Lambda M)$$

and the decompose $\Delta = \oplus_p \Delta^p$, where Δ^p is an operator of Laplace type on $C^\infty(\Lambda^p M)$.

We have $d^2 = 0$. The de Rham cohomology groups are given by taking the quotient of the closed forms by the exact forms:

$$H^p(M; \mathbb{R}) := \frac{\ker(d : C^\infty(\Lambda^p M) \to C^\infty(\Lambda^{p+1} M))}{\mathrm{im}(d : C^\infty(\Lambda^{p-1} M) \to C^\infty(\Lambda^p M))}$$

The Hodge–de Rham theorem identifies $H^p(M; \mathbb{R})$ with the kernel of the Laplacian

$$\ker(\Delta^p) = H^p(M; \mathbb{R})$$

and with the topological cohomology groups.

If ξ is a cotangent vector, let $\mathrm{e}(\xi) : \omega \to \xi \wedge \omega$ be exterior multiplication. Let $\mathrm{i}(\xi)$ be the dual operator, interior multiplication. If $\{e_i\}$ is a local

ortho-normal frame for TM, let $e^I = e^{i_1} \wedge \cdots \wedge e^{i_p}$, where $I = \{1 \le i_1 < \cdots < i_p \le m\}$. Then we have

$$\mathrm{e}(e^1)e^I = \begin{cases} 0 & \text{if } i_1 = 1 \\ e^1 \wedge e^I & \text{if } i_1 > 1 \end{cases}$$
$$\mathrm{i}(e^1)e^I = \begin{cases} e^{i_2} \wedge \cdots \wedge e^{i_p} & \text{if } i_1 = 1 \\ 0 & \text{if } i_1 > 1 \end{cases}$$

Define a Clifford module structure on ΛM by

$$\gamma(\xi) := \mathrm{e}(\xi) - \mathrm{i}(\xi)$$

If $\{e_i\}$ is a local orthonormal basis for TM, then

$$\gamma(e^i)\gamma(e^j) + \gamma(e^j)\gamma(e^i) = -2\delta_{ij}\mathrm{Id}$$

so the usual Clifford commutation rules are satisfied. Let ∇ be the Levi-Civita connection on M. We may then expand

$$d = \mathrm{e}(e^i)\nabla_{e_i}, \qquad \delta = -\mathrm{i}(e^i)\nabla_{e_i}$$
$$d + \delta = \gamma(e^i)\nabla_{e_i}$$

The de Rham complex is then defined by taking

$$\Lambda^{\text{even}}M := \oplus_k \Lambda^{2k}M, \qquad \Lambda^{\text{odd}}M := \oplus_k \Lambda^{2k+1}M$$
$$d + \delta : C^\infty(\Lambda^{\text{even}}M) \to C^\infty(\Lambda^{\text{odd}}M)$$

The Signature Complex

The signature complex arises from a different decomposition of the exterior algebra. Let Clif M be the Clifford algebra of T^*M; this is the universal unital algebra generated by T^*M subject to the Clifford commutation relations given above:

$$\xi_1 * \xi_2 + \xi_2 * \xi_1 = -2g(\xi_1, \xi_2) \cdot \mathrm{Id}$$

We suppose M is orientable and let

$$\mathrm{orn} = e_1 * \cdots * e_m \in \mathrm{Clif}\, M$$

be the orientation class. The map $\xi \to \gamma(\xi)$ extends to a unital algebra homomorphism

$$\gamma : \mathrm{Clif}\, M \to \mathrm{End}(\Lambda M)$$

$\gamma(\mathrm{orn})$ defines an endomorphism of ΛM which is, modulo suitable sign conventions, the Hodge $\star$ operator. If $m = 2k$ is even, then

$$(d + \delta)\gamma(\mathrm{orn}) = -\gamma(\mathrm{orn})(d + \delta)$$

Set

$$\Theta := (\sqrt{-1})^k\gamma(\mathrm{orn})$$

As $\Theta^2 = \mathrm{Id}$, we can decompose

$$\Lambda M \otimes \mathbb{C} = \Lambda^+ M \oplus \Lambda^- M$$

where $\Lambda^\pm M$ are the ± 1 eigenspaces of Θ. The signature complex is then given by

$$(d + \delta) : C^\infty(\Lambda^+ M) \to C^\infty(\Lambda^- M)$$

Twisted Signature Complex

Let V be an auxiliary complex vector bundle over M which is equipped with a unitary connection ∇^V. We use the connection ∇^V on V and the Levi-Civita connection on TM to covariantly differentiate tensors of all types. The twisted signature complex is defined by setting

$$(d+\delta)_V := (\gamma(e^i) \otimes \mathrm{Id})\nabla_{e_i} : C^\infty(\Lambda^+ M \otimes V) \to C^\infty(\Lambda^- M \otimes V)$$

Yang–Mills complex

This complex in dimension 4 arises from yet another decomposition of the exterior algebra. We use the discussion in the previous section to decompose

$$\Lambda^2 M = \Lambda^{2,+} M \oplus \Lambda^{2,-} M$$

into the ± 1 eigenspaces of Θ. Let

$$\pi : \Lambda^2 M \to \Lambda^{2,-} M$$

be orthogonal projection. The Yang–Mills complex is the 3-term sequence

$$d : C^\infty(\Lambda^0 M) \to C^\infty(\Lambda^1 M)$$

and

$$\pi d : C^\infty(\Lambda^1 M) \to C^\infty(\Lambda^{2,-} M)$$

We can wrap up this sequence to obtain an equivalent elliptic complex

$$(d + \delta) : C^\infty(\Lambda^{\text{even},-} M) \to C^\infty(\Lambda^{\text{odd},+} M)$$

As with the signature complex, this complex can be twisted by taking coefficients in an auxiliary vector bundle V. It is crucial to the study of four-dimensional geometry using Yang–Mills theory.

Dolbeault Complex

Let $z = (z_1, \ldots, z_k)$ be a local system of holomorphic coordinates on a complex manifold M, where $z_i = x_i + \sqrt{-1}y_i$. We define

$$dz^i := dx^i + \sqrt{-1}dy^i, \quad d\bar{z}^i := dx^i - \sqrt{-1}dy^i$$
$$\partial_i^z = \tfrac{1}{2}(\partial_i^x - \sqrt{-1}\partial_i^y), \quad \bar{\partial}_i^z = \tfrac{1}{2}(\partial_i^x + \sqrt{-1}\partial_i^y)$$

and decompose $d = \partial + \bar{\partial}$, where

$$\partial := \mathfrak{e}(\mathrm{d}z^i)\partial_i^z \quad \text{and} \quad \bar{\partial} := \mathfrak{e}(\mathrm{d}\bar{z}^i)\partial_i^{\bar{z}}$$

on the complexified exterior algebra. Let δ' be the adjoint of ∂ and δ'' be the adjoint of $\bar{\partial}$. Let

$$\mathrm{d}\bar{z}^I := \mathrm{d}\bar{z}^{i_1} \wedge \cdots \wedge \mathrm{d}\bar{z}^{i_p}$$

$$\Lambda^{(0,\mathrm{even})} := \mathrm{Span}\{\mathrm{d}\bar{z}^I\}_{|I| \text{ is even}}$$

$$\Lambda^{(0,\mathrm{odd})} := \mathrm{Span}\{\mathrm{d}\bar{z}^I\}_{|I| \text{ is odd}}$$

The Dolbeault complex is then defined by

$$(\bar{\partial} + \delta'') : C^\infty(\Lambda^{(0,\mathrm{even})}M) \to C^\infty(\Lambda^{(0,\mathrm{odd})}M)$$

This complex can be twisted by taking coefficients in a holomorphic bundle V over M.

The Spin Complex

Let M be orientable. Let P_{SO} be the principal SO bundle of orthonormal frames for the tangent bundle. A spin structure s on M is a principal Spin bundle P_{Sp} together with a double cover $\rho : P_{\mathrm{Sp}} \to P_{\mathrm{SO}}$ which respects the usual double cover $\rho : \mathrm{Spin} \to \mathrm{SO}$ of the structure groups. Equivalently, a spin structure is a lifting of the transition functions from SO to Spin which preserves the cocycle condition. One says that M is spin if it admits a spin structure.

A manifold is orientable if and only if the first Stiefel–Whitney class of M vanishes; an orientable manifold is spin if and only if the second Stiefel–Whitney class of M vanishes as well; these are $\mathbb{Z}_2$-valued cohomology classes. Inequivalent spin structures are parametrized by the cohomology group $H^1(M; \mathbb{Z}_2)$ or, equivalently, by real-line bundles on M.

The spin representation $\mathcal{S}$ of Spin defines an associated spin bundle $\mathcal{S}M = \mathcal{S}(M, s)$. There is a natural Clifford action c of TM on $\mathcal{S}M$. The Levi-Civita connection lifts to define the spin connection on $\mathcal{S}$ and the Dirac operator is defined by

$$A(s) := c(\mathrm{d}x^i)\nabla_{\partial_i^x} \quad \text{on} \quad C^\infty(\mathcal{S}M)$$

Let $m = 2k$ and let $\Theta := (\sqrt{-1})^k c(\mathrm{orn})$. Since $c(\Theta)^2 = \mathrm{Id}$, one can decompose

$$\mathcal{S}M = \mathcal{S}^+M \oplus \mathcal{S}^-M$$

as the direct sum of the half-spin bundles to obtain the spin complex:

$$A(s) : C^\infty(\mathcal{S}^+M) \to C^\infty(\mathcal{S}^-M)$$

As with the signature complex, the spin complex can be twisted by taking coefficients in an auxiliary vector bundle V.

Relating the Classic Elliptic Complexes

One has natural isomorphisms of virtual representations of the spinor group:

$$\Lambda^+ - \Lambda^- = (\mathcal{S}^+ - \mathcal{S}^-) \otimes (\mathcal{S}^+ + \mathcal{S}^-)$$
$$\Lambda^{\mathrm{even}} - \Lambda^{\mathrm{odd}} = (-1)^{m/2}(\mathcal{S}^+ - \mathcal{S}^-) \otimes (\mathcal{S}^+ - \mathcal{S}^-)$$

which show that the signature complex and de Rham complexes are the spin complexes with coefficients in the virtual bundles

$$\mathcal{S}^+M + \mathcal{S}^-M \quad \text{and} \quad (-1)^{m/2}(\mathcal{S}^+M - \mathcal{S}^-M)$$

respectively. If M is complex and spin, then the Dolbeault complex is the spin complex with coefficients in the square root of the canonical bundle.

One can consider complex spinors to define the group $\mathrm{Spin}^c(m)$. Any spin manifold admits a Spin^c structure with trivial associated complex line bundle. Any complex manifold admits a Spin^c structure with associated complex line bundle given by the canonical bundle. Thus, a complex manifold admits a Spin^c structure if and only if it is possible to take a square root of the canonical line bundle; inequivalent Spin structures are parametrized by inequivalent square roots. If M is orientable, then M admits a Spin^c structure if and only if the second Stiefel–Whitney class of M lifts from $H^2(M; \mathbb{Z}_2)$ to $H^2(M; \mathbb{Z})$; in the complex setting, this lifting is performed by the first Chern class. Inequivalent Spin^c structures are parametrized by $H^2(M; \mathbb{Z})$ or, equivalently, by complex line bundles over M.

Characteristic Classes

The Euler Form

Let ∇ be the Levi-Civita connection on M. Let

$$R(x, y) := \nabla_x \nabla_y - \nabla_y \nabla_x - \nabla_{[x,y]}$$

be the curvature operator. Let $\{e_1, \ldots, e_m\}$ be a local orthonormal frame for TM and let

$$R_{ijkl} := g(R(e_i, e_j)e_k, e_l)$$

give the components of the curvature relative to a local orthonormal frame. Let

$$\varepsilon^{I,J} := g(e^{i_1} \wedge \cdots \wedge e^{i_m}, e^{j_1} \wedge \cdots \wedge e^{j_m})$$

be the totally antisymmetric tensor; this is the sign of the permutation which sends $i_\nu \to j_\nu$. Let $m = 2\bar{m}$. The Euler form is given by setting

$$\mathcal{E}_m := \frac{1}{8^{\bar{m}}\pi^{\bar{m}}\bar{m}!}\varepsilon^{I,J} R_{i_1 i_2 j_1 j_2} \ldots R_{i_{m-1} i_m j_{m-1} j_m}$$

Let $\rho_{ij} := R_{ikkj}$ and $\tau := \rho_{ii}$ be the Ricci tensor and the scalar curvature, respectively. Then,

$$\mathcal{E}_2 = \frac{1}{4\pi}\tau \quad \text{and} \quad \mathcal{E}_4 = \frac{1}{32\pi^2}\{\tau^2 - 4|\rho|^2 + |R|^2\}$$

The Pontrjagin Forms

Since $R(x,y) = -R(y,x)$, we can regard R as a 2-form-valued endomorphism of the tangent bundle. We define the Pontrjagin forms $p_i \in C^\infty(\Lambda^{4i}M)$ by expanding

$$\det\left(I + \frac{1}{2\pi}R\right) = 1 + p_1 + p_2 + \cdots$$

These differential forms are closed and the corresponding cohomology classes

$$P_i = [p_i] \in H^{4i}(M;\mathbb{R})$$

in the de Rham cohomology are independent of the particular Riemannian metric on M which was chosen.

The $\hat{A}$ genus and the Hirzebruch L polynomial are expressed in terms of these classes using the splitting principle. Let A be a skew-symmetric matrix. One sets

$$p(A) := \det(I + A) = 1 + p_1(A) + p_2(A) + \cdots$$

As A is skew symmetric, it decomposes as the direct sum of 2×2 blocks of the form

$$\begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix}$$

We then have

$$p(A) = \prod_\nu \{1 + \lambda_\nu^2\}$$

so

$$p_i(A) = s_i(\lambda_1^2, \lambda_2^2, \ldots)$$

where s_i is the ith symmetric function;

$$p_1 = \sum_i \lambda_i^2, \qquad p_2 = \sum_{i<j} \lambda_i^2\lambda_j^2$$

and so forth. Let

$$\begin{aligned} L(\vec{\lambda}) &:= \prod_\nu \frac{\lambda_\nu}{\tanh(\lambda_\nu)} \\ &= 1 + L_1(\vec{\lambda}) + L_2(\vec{\lambda}) + \cdots \\ \hat{A}(\vec{\lambda}) &:= \prod_\nu \frac{\lambda_\nu}{2\sinh(\frac{1}{2}\lambda_\nu)} \\ &= 1 + \hat{A}_1(\vec{\lambda}) + \hat{A}_2(\vec{\lambda}) + \cdots \end{aligned}$$

As L_i and $\hat{A}_i$ are even symmetric functions of $\vec{\lambda}$, one can write $L_i = L_i(p_1(A), \ldots, p_k(A))$. For example,

$$\begin{aligned} L &= 1 + \tfrac{1}{3}p_1 + \tfrac{1}{45}(7p_2 - p_1^2) + \cdots \\ \hat{A} &= 1 - \tfrac{1}{24}p_1 + \tfrac{1}{5760}(7p_1^2 - 4p_2) + \cdots \end{aligned}$$

Substituting $(1/2\pi)R$ for A then permits one to define the Hirzebruch polynomial $L(R)$ and the $\hat{A}$ genus $\hat{A}(R)$.

The Chern Forms

Let V be a k-dimensional complex vector bundle over M. Let ∇ be a Hermitian connection on V and let Ω be the associated curvature endomorphism. The Chern forms $c_i \in C^\infty(\Lambda^{2i}M)$ are defined by expanding

$$\det\left(I + \frac{\sqrt{-1}}{2\pi}\Omega\right) = 1 + c_1 + c_2 + \cdots$$

As with the Hirzebruch polynomial and the $\hat{A}$ genus, the Chern character and Todd genus are expressed in terms of the generating functions:

$$\mathrm{Td}(\vec{\lambda}) = \prod_\nu \frac{\lambda_\nu}{1 - \mathrm{e}^{-\lambda_\nu}}$$

and

$$\mathrm{ch}(\vec{\lambda}) = \sum_\nu \frac{\lambda_\nu}{\nu!}$$

One has

$$\begin{aligned} \mathrm{Td} &= 1 + \mathrm{Td}_1 + \mathrm{Td}_2 + \cdots \\ &= 1 + \tfrac{1}{2}c_1 + \tfrac{1}{12}(c_1^2 + c_2) + \cdots \\ \mathrm{Ch} &= \mathrm{ch}_0 + \mathrm{ch}_1 + \mathrm{ch}_2 + \cdots \\ &= k + c_1 + \tfrac{1}{2}(c_1^2 - 2c_2) + \cdots \end{aligned}$$

The Index Theorem

The Gauss–Bonnet Theorem

We return to the de Rham complex. Let

$$\chi(M) = \sum_p (-1)^p \dim H^p(M;\mathbb{R})$$

be the Euler–Poincaré characteristic; $\chi(M) = 0$ if m is odd. Let M have a simplicial structure with $n(k)$ cells of degree k; $n(0)$ is the number of vertices, $n(1)$ is the number of edges, $n(2)$ is the number of triangles, etc. Then

$$\chi(M) = \sum_k (-1)^k n(k)$$

so the Euler–Poincaré characteristic is a combinatorial invariant. By the Hodge–de Rham theorem,

$$\begin{aligned}\operatorname{index}(d+\delta) &= \dim\ker(\Delta^{\text{even}}) - \dim\ker(\Delta^{\text{odd}})\\ &= \chi(M)\end{aligned}$$

The Chern–Gauss–Bonnet theorem expresses this invariant in terms of curvature

$$\chi(M) = \int_M \mathcal{E}_m \,\mathrm{d}x$$

where $\mathcal{E}_m$ is the Euler form given above. If one twists the de Rham complex to take coefficients in an auxiliary vector bundle V, then no new information results, since

$$\operatorname{index}\{d+\delta\}_V = \chi(M)\cdot\dim(V)$$

The Hirzebruch Signature Theorem

Let sign (M) be the index of the signature complex on a manifold of dimension $4k$; the index vanishes in dimensions $m \equiv 2 \bmod 4$. Let $\star$ be the Hodge duality operator. As $\star\Delta^p\star^{-1} = \Delta^{m-p}$, $\star$ preserves the eigenspaces of the Laplacian. In particular, $\star$ induces an isomorphism

$$\begin{aligned}\star : H^p(M;\mathbb{R}) &= \ker(\Delta^p)\\ \to H^{m-p}(M;\mathbb{R}) &= \ker(\Delta^{m-p})\end{aligned}$$

which implements Poincaré duality. In dimension $2k$, $\star^2 = \mathrm{Id}$. Decompose

$$H^{2k}(M;\mathbb{R}) = H^{2k,+}(M;\mathbb{R}) \oplus H^{2k,-}(M;\mathbb{R})$$

into the ±1 eigenspaces of $\star$; these may be identified with $\ker(\Delta^{2k,\pm})$ acting on $C^\infty(\Lambda^{2k,\pm}M)$. As the contributions to the signature away from the middle dimension cancel,

$$\operatorname{sign}(M) = \dim H^{2k,+}(M;\mathbb{R}) - \dim H^{2k,-}(M;\mathbb{R})$$

As with the de Rham complex, there is a topological description of this invariant. If α and β are closed $2k$ forms, one sets

$$\langle\alpha,\beta\rangle := \int_M \alpha\wedge\beta$$

One can use Stoke's theorem to see that this induces a symmetric bilinear form on the de Rham cohomology groups $H^{2k}(M;\mathbb{R})$. Poincaré duality then shows that this symmetric bilinear form is nondegenerate, so this is a form of type (p,q); $\operatorname{sign}(M)$ is the signature of this quadratic form:

$$\operatorname{sign}(M) = q - p$$

The Hirzebruch signature formula expresses sign (M) in terms of curvature; if L is the Hirzebruch polynomial described above and if $m = 4k$, then

$$\operatorname{sign}(M) = \int_M L_k$$

Let V be an auxiliary coefficient bundle. Taking coefficients in V then yields the formula

$$\operatorname{sign}_V(M) = \sum_{4i+2j=m} 2^j \int_M L_i \wedge \operatorname{ch}_j(V)$$

The Index of the Yang–Mills Complex

Let YM_V be the Yang–Mills complex with coefficients in an auxiliary vector bundle V, then the index can be evaluated using the formulas given above as

$$\begin{aligned}\operatorname{index}\{\mathrm{YM}_V\} &= \tfrac{1}{2}\{\dim(V)\chi(M) - \operatorname{sign}(M,V)\}\\ &= \tfrac{1}{2}\textstyle\int_M\{\dim V\mathcal{E}_4 - \dim VL_1 - 4\operatorname{ch}_2(V)\}\end{aligned}$$

The Index of the Dolbeault Complex

If V is a holomorphic bundle over a complex manifold M, then

$$\operatorname{index}\{(\bar\partial+\delta'')_V\} = \sum_{2i+2j=m}\int_M \operatorname{Td}_i(M)\wedge\operatorname{ch}_j(V)$$

The index of the untwisted Dolbeault complex is called the arithmetic genus and denoted by $\operatorname{ag}(M)$.

The Index of the Spin Complex

If M is a spin manifold and if A_V is the Dirac operator with coefficients in an auxiliary coefficient bundle, then

$$\operatorname{index}\{A_V\} = \sum_{4i+2j=m}\int_M \hat{A}_i(M)\wedge\operatorname{ch}_j(M)$$

The index of the spin complex is called the $\hat{A}$ genus and is denoted by $\hat{A}(M)$. If M is a Spin^c manifold, the appropriate formula becomes

$$\operatorname{index}\{A_V^c\} = \sum_{4i+2j+2k=m}\int_M \hat{A}_i(M)\wedge\operatorname{ch}_j(M)\wedge\theta^k$$

where $\theta = \frac{1}{2}c_1(L)$, L being the complex line bundle associated with the Spin^c structure.

Properties

The classic elliptic complexes defined above are multiplicative with respect to Cartesian product. Suppose that M_1 and M_2 are Riemannian manifolds with the appropriate structures. For the signature complex, suppose M_1 and M_2 are oriented; for the Dolbeault complex, suppose M_1 and M_2 are holomorphic; for the spin complex, suppose M_1 and M_2 are spin. By taking the twisting coefficient bundle to be trivial in the interests of simplicity, one has

$$\chi(M_1 \times M_2) = \chi(M_1)\chi(M_2)$$
$$\mathrm{sign}(M_1 \times M_2) = \mathrm{sign}(M_1)\mathrm{sign}(M_2)$$
$$\mathrm{ag}(M_1 \times M_2) = \mathrm{ag}(M_1)\mathrm{ag}(M_2)$$
$$\hat{A}(M_1 \times M_2) = \hat{A}(M_1)\hat{A}(M_2)$$

These complexes behave well under finite coverings. Let $F \to M_2 \to M_1$ be a finite covering projection with $|F|$ sheets. Then

$$\chi(M_2) = |F|\chi(M_1)$$
$$\mathrm{sign}(M_2) = |F|\mathrm{sign}(M_1)$$
$$\mathrm{ag}(M_2) = |F|\mathrm{ag}(M_1)$$
$$\hat{A}(M_2) = |F|\hat{A}(M_1)$$

The connected sum $M_1\#M_2$ is defined by punching out small disks about points P_i in M_i and then joining along the spherical boundaries that remain. It is necessary, of course, to smooth out the resulting corners. Note that if M_1 and M_2 are complex manifolds, then $M_1\#M_2$ is no longer a complex manifold in general. Since

$$\chi(S^m) = 2, \quad \mathrm{sign}(S^m) = 0, \text{ and } \hat{A}(S^m) = 0$$

the following additivity results follow from the integral formulas given above:

$$\chi(M_1\#M_2) = \chi(M_1) + \chi(M_2) - 2$$
$$\mathrm{sign}(M_1\#M_2) = \mathrm{sign}(M_1) + \mathrm{sign}(M_2)$$
$$\hat{A}(M_1\#M_2) = \hat{A}(M_1) + \hat{A}(M_2)$$

Examples and Applications

Let S^m be the standard sphere and let $\mathbb{CP}^j$ be the complex projective plane. One then has

$$\chi(S^4) = 2, \qquad \mathrm{sign}(S^4) = 0$$
$$\chi(S^2 \times S^2) = 4, \quad \mathrm{sign}(S^2 \times S^2) = 0$$
$$\chi(\mathbb{CP}^2) = 3, \qquad \mathrm{sign}(\mathbb{CP}^2) = 1$$

In dimension 4, the Riemann–Roch formula yields

$$\mathrm{ag}(M^4) = \tfrac{1}{4}\{\chi(M) + \mathrm{sign}(M)\}$$

This would yield $\mathrm{ag}(S^4) = \frac{1}{2}$; since $\frac{1}{2}$ is not an integer, this shows that S^4 does not admit a complex structure; a similar argument shows that S^n does not admit a complex structure for $n \neq 2, 6$, and it is not known whether S^6 admits a holomorphic structure; it does admit an almost-complex structure.

If we set $M = \mathbb{CP}^2\#\mathbb{CP}^2$, then

$$\mathrm{ag}(M) = \tfrac{1}{4}(3 + 3 - 2 + 1 + 1) = \tfrac{3}{2}$$

and thus $\mathbb{CP}^2\#\mathbb{CP}^2$ does not admit a complex structure. These examples are typical of the use of the index theorem to prove the nonexistence of certain structures.

The General Index Theorem

Let $S(T^*M)$ be the sphere bundle of unit cotangent vectors and let $D(T^*M)$ be the disk bundle of cotangent vectors of length at most 1. Let

$$P : C^\infty(V_1) \to C^\infty(V_2)$$

be an elliptic pseudodifferential operator. The leading symbol $p := \sigma_L(P)$ induces a smooth map

$$p : S(T^*M) \to \mathrm{End}(V_1, V_2).$$

We form $\Sigma(M)$ by gluing two copies of $D(M)$ together along their common boundary $S(M)$ and we define a bundle $\Sigma(p, V_1, V_2)$ over $\Sigma(M)$ by gluing V_1 to V_2 over $S(M)$ using the clutching function p. The Atiyah–Singer index theorem expresses the index of P in terms of cohomological data involving the Chern class of the symbol bundle and the characteristic classes of the tangent bundle of M. If $\Sigma(M)$ is given a suitable orientation, then

$$\mathrm{index}(P) = \sum_{2i+4j=2m} \int_{\Sigma(M)} \mathrm{ch}_i(\Sigma(p, V_1, V_2)) \wedge \mathrm{Td}_j(M)$$

It specializes to the results given above for the classical elliptic complexes. Conversely, by using K-theoretic methods, the index theorem in full generality can be derived from the special case of the twisted signature complex.

Manifolds with Boundary

If the boundary of M is nonempty, we must impose suitable boundary conditions.

Local Boundary Conditions

Choose local coordinates $x = (x^1, \ldots, x^m)$ near the boundary of M so that x^m is the geodesic distance to the boundary. On the boundary, we can decompose a differential form $\omega \in C^\infty(\Lambda M)$ in the form $\omega = \omega_1 + \mathrm{d}x^m \wedge \omega_2$, where ω_1 and ω_2 are tangential

differential forms. Absolute and relative boundary conditions are defined by setting

$$\mathcal{B}_a\omega := \omega_2|_{\partial M} \quad \text{and} \quad \mathcal{B}_r\omega := \omega_1|_{\partial M}$$

Let $(d+\delta)_a$ and $(d+\delta)_r$ be the associated realizations. These operators preserve the grading of the exterior algebra $\Lambda M = \Lambda^{\text{even}}M \oplus \Lambda^{\text{odd}}M$ and define elliptic complexes

$$(d+\delta)_a : C^\infty(\Lambda^{\text{even}}M) \to C^\infty(\Lambda^{\text{odd}}M)$$
$$(d+\delta)_r : C^\infty(\Lambda^{\text{even}}M) \to C^\infty(\Lambda^{\text{odd}}M)$$

We consider a collection

$$J = \{1 \le j_1 < \cdots < j_p < m\}$$

of tangential indices and let

$$dx^J = dx^{j_1} \wedge \cdots \wedge dx^{j_p}$$

The associated absolute boundary conditions for the Laplacian are defined by

$$\begin{aligned}&\tilde{\mathcal{B}}_a(\phi_J dx^J + \psi_J dx^m \wedge dx^J)\\&\quad = (\psi_J|_{\partial M} dx^J) \oplus (\partial_m^x \phi_J|_{\partial M}) dx^J\end{aligned}$$

If $\star$ is the Hodge operator, then one sets dually:

$$\tilde{\mathcal{B}}_r(\omega) = \tilde{\mathcal{B}}_a(\star\omega)$$

Let Δ_a^p and Δ_r^p be the associated realizations of the Laplacian with these boundary conditions. The Hodge–de Rham theorem extends to this setting to yield isomorphisms

$$\ker(\Delta_a^p) = H^p(M;\mathbb{R})$$

and

$$\ker(\Delta_r^p) = H^p(M, \partial M;\mathbb{R})$$

The Hodge $\star$ operator intertwines Δ_a^p and Δ_r^{m-p} and implements the Poincaré duality isomorphism $H^p(M;\mathbb{R}) = H^{m-p}(M, \partial M;\mathbb{R})$. This also shows that

$$\text{index}(d+\delta)_a = \sum_p (-1)^p \dim H^p(M;\mathbb{R}) = \chi(M)$$

and

$$\begin{aligned}\text{index}(d+\delta)_r &= \sum_p (-1)^p \dim H^p(M, \partial M;\mathbb{R})\\&= \chi(M, \partial M) = \chi(M) - \chi(\partial M)\end{aligned}$$

Let $\mathcal{E}_m$ be the Euler form if m is even. We set $\mathcal{E}_m = 0$ if m is odd. Let L be the second fundamental form. Let $A = (a_1, \ldots, a_{m-1})$ and $B = (b_1, \ldots, b_{m-1})$ be collections of distinct indices ranging from 1 to $m-1$. Set

$$\begin{aligned}\mathcal{L}_{m-1} := \sum_k & \frac{1}{\pi^k 8^k k!(m-1-2k)!\text{vol}(S^{m-1-2k})}\\&\times \varepsilon^{A,B} R_{a_1a_2b_2b_1} \ldots R_{a_{2k-1}a_{2k}b_{2k}b_{2k-1}}\\&\times L_{a_{2k+1}b_{2k+1}} \ldots L_{a_{m-1}b_{m-1}}\end{aligned}$$

The Chern–Gauss–Bonnet theorem generalizes to this setting to yield

$$\begin{aligned}\chi(M) &= \text{index}(d+\delta)_a\\&= \int_M \mathcal{E}_m \text{d}x + \int_{\partial M} \mathcal{L}_{m-1} \text{d}y\end{aligned}$$

For example,

$$\begin{aligned}\chi(M^2) &= \frac{1}{4\pi}\left\{\int_{M^2} \tau \text{d}x + 2\int_{\partial M^2} L_{aa} \text{d}y\right\}\\ \chi(M^3) &= \frac{1}{8\pi}\int_{\partial M^3} \{R_{abba} + L_{aa}L_{bb} - L_{ab}L_{ab}\} \text{d}y\\ \chi(M^4) &= \frac{1}{32\pi^2}\int_{M^4} \{\tau^2 - 4|\rho|^2 + |R|^2\} \text{d}x\\&\quad + \frac{1}{24\pi^2}\int_{\partial M^4} \{3\tau L_{aa} + 6R_{amam}L_{bb}\\&\quad + 6R_{acbc}L_{ab} + 2L_{aa}L_{bb}L_{cc}\\&\quad - 6L_{ab}L_{ab}L_{cc} + 4L_{ab}L_{bc}L_{ac}\} \text{d}y\end{aligned}$$

The interior integral vanishes if m is odd. The boundary integral can be nonzero in any dimensions. Thus, in particular, the index of this elliptic complex can be nonzero even if m is odd; $\chi(D^m) = 1$ for any m. The index of $(d+\delta)_r$ is computed similarly.

Spectral Boundary Conditions

In contrast to the de Rham complex, there do not exist local boundary conditions for the signature, spin, and Dolbeault complexes. To simplify the discussion, we assume that the metric is the product near the boundary; there are appropriate compensating terms involving the second fundamental form in the more general setting. Let $A : C^\infty(V_1) \to C^\infty(V_2)$ denote either the twisted signature or the twisted spin complexes; there are some additional difficulties for the Dolbeault complex. Near the boundary, we can express

$$A = \sigma(\partial_m^x + A_{\text{T}})$$

where A_{T} is a self-adjoint tangential operator of Dirac type on $V_1|_{\partial M}$ and σ is a unitary bundle

isomorphism from $V_1|_{\partial M}$ to $V_2|_{\partial M}$. Let $\{\phi_i, \lambda_i\}$ be the discrete spectral resolution of A_{T}. One defines

$$\eta(A_{\mathrm{T}}, s) = \sum_{\lambda_k \neq 0} \mathrm{sgn}(\lambda_k)|\lambda_k|^{-s}$$

as a measure of the spectral asymmetry of A_{T}. This is well defined for $\mathrm{Re}(s) \gg 1$ and has a meromorphic extension to the complex plane $\mathbb{C}$. It turns out that 0 is a regular value and one defines

$$\eta(A_T) := \tfrac{1}{2}\{\eta(A_{\mathrm{T}}, s) + \dim \ker(A_{\mathrm{T}})\}|_{s=0}$$

The spectral boundary conditions can now be imposed. Let $\Pi_{\geq}$ be orthogonal projection in $L^2(V_1|_{\partial M})$ on the span of the eigensections of A_{T} corresponding to non-negative eigenvalues and let $A_{\geq}$ be the associated realization defined by this boundary condition.

One can use the Atiyah–Patodi–Singer index theorem to generalize the relations given above to this setting. Let f_A be the local integral given above that involves the Hirzebruch L polynomial for the signature complex or the $\hat{A}$ genus for the spin complex. One then has

$$\mathrm{index}(A_{\geq}) = \eta(A_{\mathrm{T}}) + \int_M f_A$$

There are suitable correction formulas involving integrals of polynomials in the second fundamental form and in the curvature tensor if the structures are not product near the boundary.

Equivariant Problems

The Classical Lefschetz Formula

Let M be a compact Riemannian manifold without boundary. Let T be a smooth map from M to M. Then pullback T^* induces an action on $C^\infty(\Lambda^p M)$ which commutes with the exterior derivative d and hence an action on the de Rham cohomology groups $H^p(M; \mathbb{R})$. The Lefschetz number of T is then given by

$$\mathcal{L}(T) = \sum_p (-1)^p \mathrm{tr}\{T^* \text{ on } H^p(M; \mathbb{R})\}$$

To illustrate the Lefschetz number, let $M = \mathbb{T}^2$ be the two-dimensional torus. Let $e^1 := \mathrm{d}x^1$, let $e^2 := \mathrm{d}x^2$, and let $e^{12} := \mathrm{d}x^1 \wedge \mathrm{d}x^2$. Then,

$$\begin{aligned} H^0(\mathbb{T}^2; \mathbb{R}) &= 1 \cdot \mathbb{R} \\ H^1(\mathbb{T}^2; \mathbb{R}) &= e^1 \cdot \mathbb{R} + e^2 \cdot \mathbb{R} \\ H^2(\mathbb{T}^2; \mathbb{R}) &= e^{12} \cdot \mathbb{R} \end{aligned}$$

Let $T(x_1, x_2) = (n_{11}x_1 + n_{12}x_2,\ n_{21}x_1 + n_{22}x_2)$. Then,

$$\begin{aligned} T^*(1) &= 1 \\ T^*(e^1) &= n_{11}e^1 + n_{12}e^2 \\ T^*(e^2) &= n_{21}e^1 + n_{22}e^2 \\ T^*(e^{12}) &= (n_{11}n_{22} - n_{12}n_{21})e^{12} \end{aligned}$$

and, consequently, the Lefschetz number becomes

$$\begin{aligned} \mathcal{L}(T) &= \det(I - T^*) \\ &= 1 - (n_{11} + n_{22}) + (n_{11}n_{22} - n_{12}n_{21}) \end{aligned}$$

The classical Lefschetz fixed-point formula expresses $\mathcal{L}$ in terms of data for the fixed-point set $\mathcal{F}(T)$ and is an example of the equivariant index theorem. One assumes that the fixed-point set of T consists of smooth submanifolds $N_1, \ldots, N_k$ and that the induced map $\mathrm{d}T_\nu$ on the normal bundles of these manifolds is nondegenerate. This means that $\det(I - \mathrm{d}T_\nu) \neq 0$, that is, that there are no infinitesimal normal directions which are left fixed. One then has

$$\mathcal{L}(T) = \sum_i \mathrm{sign}(\det(I - \mathrm{d}T_\nu))\chi(N_i)$$

The Lefschetz Formula for the Other Classical Elliptic Complexes

Let T be an orientation-preserving isometry of M. When dealing with the spin complex, suppose that T preserves the spin structure; when dealing with the Dolbeault complex, suppose that T preserves the holomorphic structure. If

$$A : C^\infty(V_1) \to C^\infty(V_2)$$

is one of the classical elliptic complexes, then by assumption T^* commutes with A and hence preserves the eigenspaces of the associated Laplacians. The Lefschetz number is defined by setting

$$\begin{aligned} \mathcal{L}_A(T) := &\mathrm{tr}(T^* \text{ on } \ker(A^*A)) \\ &- \mathrm{tr}(T^* \text{ on } \ker(AA^*)) \end{aligned}$$

Setting $T = \mathrm{Id}$, one recovers the standard index.

To simplify the discussion, we assume henceforth that T is an orientation-preserving isometry of M with only isolated fixed points. Let $\{\theta_1, \ldots, \theta_{m/2}\}$ be the rotation angles of $\mathrm{d}T$ at a fixed point x of T. Set

$$\lambda_j := \cos(\theta_j) + \sqrt{-1}\sin(\theta_j)$$

We take the sum over the isolated fixed points x and then the product over the rotation angles $1 \leq j \leq m/2$ to express

$$\mathcal{L}_{\mathrm{sign}}(T) = \sum_x \prod_j \left\{ -\sqrt{-1} \cot\left(\frac{\theta_j}{2}\right) \right\}$$
$$\mathcal{L}_{\mathrm{spin}}(T) = \sum_x \prod_j \left\{ -\frac{1}{2}\sqrt{-1} \csc\left(\frac{\theta_j}{2}\right) \right\}$$
$$\mathcal{L}_{\mathrm{Dolb}}(T) = \sum_x \prod_j (1 - \bar{\lambda}_j)^{-1}$$

In considering the spin complex, we assume T preserves the spin structure. This permits us to lift $\mathrm{d}T$ from $\mathrm{SO}(m)$ to $\mathrm{Spin}(m)$ and defines liftings of the rotation angles θ_j from $[0, 2\pi]$ to $[0, 4\pi]$ in such a way that the formula given above for the spin complex is well defined. In considering the Dolbeault complex, we assume that T preserves a complex structure, so the formula given above for the Dolbeault complex involving the complex eigenvalues λ_j is well defined.

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See also: Anomalies; Clifford Algebras and their Representations; Cohomology Theories; Dirac Operator and Dirac Field; Gerbes in Quantum Field Theory; Intersection Theory; Instantons: Topological Aspects; K-Theory; Path-Integrals in Non Commutative Geometry; Quillen Determinant; Riemann Surfaces; Spinors and Spin Coefficients.

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Inequalities in Sobolev Spaces

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Introduction

Given $1 \le p < n$, it was shown by Sobolev that there exists a constant $K > 0$ such that, for any $u \in C_0^\infty(\mathbb{R}^n)$, the space of smooth functions with compact support in $\mathbb{R}^n$,

$$\left(\int_{\mathbb{R}^n} |u|^{p^\star} \mathrm{d}x \right)^{1/p^\star} \le K \left(\int_{\mathbb{R}^n} |\nabla u|^p \mathrm{d}x \right)^{1/p} \qquad [1]$$

where ∇u is the gradient of u and $p^\star = np/(n-p)$. It is easily seen that $p^\star$ in [1] is critical in the following sense. Let $\|\cdot\|_p$ stand for the L^p-norm. For $u \in C_0^\infty(\mathbb{R}^n)$, and $\lambda > 0$, let also u_λ be the function given by $u_\lambda(x) = u(\lambda x)$. For p and q two real numbers,

$$\|\nabla u_\lambda\|_p = \lambda^{1-(n/p)} \|\nabla u\|_p$$
$$\|u_\lambda\|_q = \lambda^{-n/q} \|u\|_q$$

Letting $\lambda \to 0$ and $\lambda \to +\infty$, it follows that an inequality like $\|u\|_q \le K\|\nabla u\|_p$ holds true for all u (in particular for the u_λ's) only when $q = p^\star$. To

prove [1], the approach of Sobolev was based on the straightforward representation formula

$$u(x) = -\frac{\Gamma(n/2)}{2\pi^{n/2}}\int_{\mathbb{R}^n}\sum_{k=1}^{n}\frac{x^k - y^k}{|x-y|^n}\partial_k u(y)\mathrm{d}y$$

where Γ is the Gamma function, and on an n-dimensional version of a theorem of Hardy–Littlewood concerning fractional integrals that we apply to the right-hand side of the above representation formula. More direct arguments were later discovered in independent works by Gagliardo and Nirenberg. In particular, the explicit inequality

$$\left(\int_{\mathbb{R}^n}|u|^{n/(n-1)}\mathrm{d}x\right)^{(n-1)/n} \le \frac{1}{2}\prod_{k=1}^{n}\left(\int_{\mathbb{R}^n}|D_k u|\mathrm{d}x\right)^{1/n} \le \frac{1}{2}\int_{\mathbb{R}^n}|\nabla u|\mathrm{d}x \qquad [2]$$

was proved to hold, where D_k is the partial derivative $D_k=\partial/\partial x_k$. Inequality [2] is of the form [1] when $p=1$, since $1^\star = n/(n-1)$. By geometric measure theory, and the coarea formula, it can be expressed as an isoperimetric type inequality.

There have been several symbols and several definitions for Sobolev spaces. Before they became generally associated with the name of Sobolev, they were sometimes referred to by other names, for instance, as "Beppo Levi spaces." We often find two definitions and two notations in the literature. For Ω a domain in $\mathbb{R}^n, p \ge 1$ real, and u of class C^m in Ω, we let

$$\|u\|_{m,p} = \left(\sum_{0\le|\alpha|\le m}\|D^\alpha u\|_p^p\right)^{1/p} \qquad [3]$$

when the right-hand side makes sense, where $\|\cdot\|_p$ is the L^p-norm, $\alpha=(\alpha_1,\ldots,\alpha_n)$ is a multi-index, $|\alpha| = \sum_i \alpha_i$, and $D^\alpha = D_1^{\alpha_1}\cdots D_n^{\alpha_n}$. We define

$$H^{m,p}(\Omega) = \text{the completion of } \{u\in C^m(\Omega) \text{ s.t. } \|u\|_{m,p} < +\infty\} \text{ with respect to the norm } \|\cdot\|_{m,p}$$

$$W^{m,p}(\Omega) = \{u \in L^p(\Omega) \text{ s.t. } D^\alpha u \in L^p(\Omega) \text{ for all } 0 \le |\alpha| \le m\}$$

where D^α is the weak (or distributional) partial derivative of u with respect to the multi-index α. Both $H^{m,p}(\Omega)$ and $W^{m,p}(\Omega)$ are Banach spaces (and even Hilbert when $p=2$). It is easily seen that $H^{m,p}(\Omega) \subset W^{m,p}(\Omega)$, but we had to wait for the work of Meyers and Serrin to realize that $H^{m,p}(\Omega) = W^{m,p}(\Omega)$. The spaces $H^{m,p}(\Omega)$, also denoted $W^{m,p}(\Omega)$, are referred to as Sobolev spaces. The spaces $H_0^{m,p}(\Omega)$, also denoted $W_0^{m,p}(\Omega)$, are defined as the closure of $C_0^\infty(\Omega)$ in $H^{m,p}(\Omega)$, where $C_0^\infty(\Omega)$ is the space of smooth functions with compact support in Ω.

Inequality [1] states that the Sobolev space $H_0^{1,p}(\mathbb{R}^n)$ is naturally embedded in the Lebesgue space $L^{p^\star}(\mathbb{R}^n)$, a particular case of what we now refer to as Sobolev embeddings.

Sobolev Inequalities and the Sobolev Embedding Theorem in Its First Part

Let m be an integer and let $p\ge 1$ be real. The Sobolev space $H^{m,p}(\mathbb{R}^n)$, also denoted by $W^{m,p}(\mathbb{R}^n)$, is defined by in one of the two equivalent ways:

$$H^{m,p}(\mathbb{R}^n) = \text{the completion of } \{u\in C^m(\mathbb{R}^n) \text{ s.t. } \|u\|_{m,p} < +\infty\} \text{ with respect to the norm } \|\cdot\|_{m,p}$$

or

$$H^{m,p}(\mathbb{R}^n) = \{u \in L^p(\mathbb{R}^n) \text{ s.t. } D^\alpha u \in L^p(\mathbb{R}^n) \text{ for all } 0 \le |\alpha| \le m\}$$

where D^α is the weak (or distributional) partial derivative of u with respect to the multi-index α, and $\|\cdot\|_{m,p}$ is as in [3]. The Sobolev space $(H^{m,p}(\mathbb{R}^n), \|\cdot\|_{m,p})$ is a Banach space, and even a Hilbert space when $p=2$. The space is reflexive when $p>1$, and we also have that $H^{m,p}(\mathbb{R}^n) = H_0^{m,p}(\mathbb{R}^n)$, where $H_0^{m,p}(\mathbb{R}^n)$ is defined as the closure of $C_0^\infty(\mathbb{R}^n)$ in $H^{m,p}(\mathbb{R}^n)$. What we usually refer to as the first part of Sobolev inequalities can be expressed as follows.

Sobolev embeddings (*Part I*). For p, q two real numbers with $1\le q<p$, and k, m two integers with $0\le m<k$, if $1/p = 1/q-(k-m)/n$, then $H^{k,q}\subset H^{m,p}$, and there exists $K>0$ such that $\|u\|_{m,p}\le K\|u\|_{k,q}$ for all $u\in H^{k,q}$.

The Sobolev theorem in its first part states that the above Sobolev embeddings (resp. inequalities) hold true for the Euclidean space. A particular case of interest is when $k=1$. In this case, we get, as in the introduction, that for any $1\le p<n, H^{1,p}(\mathbb{R}^n)\subset L^{p^\star}(\mathbb{R}^n)$ where $p^\star = np/(n-p)$. The embedding for the Euclidean space reduces to the Sobolev inequality [1]. An important remark is that there is a hierarchy for Sobolev embeddings. In particular, that if $H^{1,1}\subset L^{n/(n-1)}, 1^\star = n/(n-1)$, then all the other embeddings $H^{k,q}\subset H^{m,p}$ hold true. Thanks to this remark, the Sobolev embedding theorem for Euclidean space easily follows from an inequality like [2]. The hierarchy for Sobolev embeddings is an easy consequence of Hölder's inequalities when $k=1$, and of Hölder's inequalities together with Kato's inequality when $k>1$.

There are several extensions of Sobolev inequalities in the literature. Famous extensions were discovered by Gagliardo and Nirenberg. The Nash inequality, which reads as

$$\left(\int_{\mathbb{R}^n} u^2\,dx\right)^{(n+2)/n} \leq K\left(\int_{\mathbb{R}^n} |u|\,dx\right)^{4/n} \times \int_{\mathbb{R}^n} |\nabla u|^2\,dx \qquad [4]$$

for all $u \in H^{1,2}(\mathbb{R}^n)$, is one of the Gagliardo–Nirenberg's inequalities. The Nash inequality easily follows from [1] when $p = 2$ and Hölder's inequality. There are also extensions of Sobolev spaces, for instance, spaces of BV-functions or Orlicz–Sobolev spaces.

The Sobolev Embedding Theorem in Its Second Part

For m integer, let $C_B^m(\mathbb{R}^n)$ be the space of functions of class C^m in $\mathbb{R}^n$ for which the norm

$$\|u\|_{C^m} = \sum_{0\leq|\alpha|\leq m} \sup_{x\in\mathbb{R}^n} |D^\alpha u(x)|$$

is finite. What we usually refer to as the second part of Sobolev inequalities can be expressed as follows.

Sobolev embeddings (*Part II*). For $q \geq 1$ a real number, and k, m two integers with $0 \leq m < k$, if $1/q - (k-m)/n < 0$, then $H^{k,q} \subset C_B^m$, and there exists $K > 0$ such that $\|u\|_{C^m} \leq K\|u\|_{k,q}$ for all $u \in H^{k,q}$.

The Sobolev theorem in its second part states that the above Sobolev embeddings (resp. inequalities) hold true for the Euclidean space. Refinements were then obtained by Morrey with embeddings in Hölder spaces. Let, for instance, $C^{0,\alpha}(\mathbb{R}^n)$ be the Hölder space of continuous functions in $\mathbb{R}^n$ for which the norm

$$\|u\|_{C^{0,\alpha}} = \sup_{x\in\mathbb{R}^n} |u(x)| + \sup_{x\neq y} \frac{|u(y)-u(x)|}{|y-x|^\alpha}$$

is finite. For $k = 1, m = 0$, and $q \geq 1$ such that $1/q - 1/n < 0$, the embedding $H^{1,q}(\mathbb{R}^n) \subset C_B^0(\mathbb{R}^n)$ can be refined into an embedding like $H^{1,q}(\mathbb{R}^n) \subset C^{0,\alpha}(\mathbb{R}^n)$, where $\alpha \in (0,1)$ is such that $1/q - (1-\alpha)/n < 0$.

The Case of Domains and the Kondrakov Theorem

The Sobolev embeddings in their first and second parts extend to regular domains Ω. A typical condition is that Ω satisfies a cone property. When Ω is bounded, and thus of finite volume, an embedding like $H^{1,p}(\Omega) \subset L^{p^*}(\Omega)$ implies that we also have that $H^{1,p}(\Omega) \subset L^q(\Omega)$ for all $1 \leq q \leq p^\star$. The Kondrakov theorem states that such embeddings are all compact, unless $q = p^\star$, in the sense that bounded sequences of functions in $H^{1,p}$ possess converging subsequences in L^q.

For $p \geq 1$ real, the Sobolev embedding theorem in its first part provides embeddings of $H^{1,p}$ into Lebesgue spaces when $p < n$, while the Sobolev embedding theorem in its second part provides embeddings of $H^{1,p}$ into Hölder spaces when $p > n$. For $p = n$, it is false that $H^{1,n}$ can be embedded into L^∞. However, when Ω is bounded, we can prove that $\exp(u) \in L^1(\Omega)$ when $u \in H_0^{1,n}(\Omega)$, and that

$$\int_\Omega \exp(u)\,dx \leq K\exp(\mu\|u\|_{1,n}^n)$$

where $\mu, K > 0$ are independent of u. We also have that

$$\int_\Omega \exp(\mu|u|^{n/(n-1)})\,dx \leq K$$

for all $u \in H_0^{1,n}(\Omega)$ such that $\|\nabla u\|_n \leq 1$, where μ, $K > 0$ are independent of u. Such inequalities are often referred to as Moser–Trüdinger type inequalities.

The Case of Riemannian Manifolds

Riemannian manifolds are natural extensions of Euclidean space. For (M, g) a Riemannian manifold, m integer, and $p \geq 1$ real, we define the Sobolev space $H^{m,p}(M)$ by

$$H^{m,p}(M) = \text{the completion of } \{u \in C^m(M) \text{ s.t. } \|u\|_{m,p} < +\infty\} \text{ with respect to the norm } \|\cdot\|_{m,p}$$

where $\|u\|_{m,p} = \sum_{i=0}^m \|\nabla^i u\|_p$, $\nabla^i u$ is the ith covariant derivative of u, and $\|\cdot\|_p$ is the L^p-norm in (M, g). A notation like $\|\nabla^i u\|_p$ stands for the L^p-norm of the pointwise norm $|\nabla^i u|$ of $\nabla^i u$. Sobolev spaces on manifolds are Banach spaces, even Hilbert when $p = 2$, and they are reflexive when $p > 1$. They do not depend on the metric when M is compact.

For compact Riemannian manifolds, everything works as for bounded domains. The Sobolev embeddings in their first and second parts remain valid. The Kondrakov theorem also remains valid. However, since constant functions are in Sobolev spaces when the manifold is compact, the L^p-norm of u in the $H^{1,p}$-norm of u should be added to the right-hand side in inequalities like [1]. More precisely, if (M,g) is a compact Riemannian

manifold of dimension n, and $1 \le p < n$, then the inequality for the embedding $H^{1,p}(M) \subset L^{p^*}(M)$ reads as: there exists $K > 0$ such that for any $u \in H^{1,p}(M)$,

$$\left(\int_M |u|^{p^*} dv_g\right)^{p/p^*} \le K\left(\int_M |\nabla u|^p dv_g + \int_M |u|^p dv_g\right) \quad [5]$$

where dv_g is the Riemannian volume element with respect to g. When (M, g) is no longer compact, the Sobolev embedding theorem might become false. A nontrivial key observation is that a Sobolev inequality like [5] on a complete manifold (M, g) implies the existence of a uniform (with respect to the center) lower bound for the volume of balls of radius 1. It follows that for any $n \ge 2$, there exist complete Riemannian n-manifolds (M, g) for which, for any $p \in [1, n), H^{1,p}(M) \not\subset L^{p^*}(M)$. Possible examples are warped products of the real line $\mathbb{R}$ and the $(n-1)$-sphere S^{n-1}. When the Ricci curvature is bounded from below, the condition that there is a uniform (with respect to the center) lower bound for the volume of balls of radius 1 is necessary and sufficient in order to get that the Sobolev embeddings are valid.

Isoperimetric and Euclidean Type Inequalities

Let (M, g) be a complete Riemannian n-manifold. Euclidean type inequalities are said to hold on (M, g) if there exists $K > 0$ such that for any $1 \le p < n$, and any $u \in H^{1,p}(M)$,

$$\left(\int_M |u|^{p^*} dv_g\right)^{1/p^*} \le K\left(\int_M |\nabla u|^p dv_g\right)^{1/p} \quad [6]$$

where $p^* = np/n - p$. As for the Euclidean space, if the above inequality holds for some p_0, then it holds, with distinct K, for all $p_0 \le p < n$. In particular, if the inequality holds for $p = 1$, it holds for all p's. The inequality when $p = 1$ was shown to be true by Hoffman and Spruck when the manifold is simply connected of nonpositive sectional curvature. Such manifolds are referred to as Cartan–Hadamard manifolds. The inequality when $p = 2$ is related to the nonparabolicity of the manifold, namely the existence of a minimal Green's function, and to the behavior of the minimal Green's function.

By geometric measure theory and the coarea formula, [6] when $p = 1$ is equivalent to the isoperimetric inequality

$$\text{Area}_g(\partial\Omega) \ge \frac{1}{C}\text{Vol}_g(\Omega)^{(n-1)/n} \quad [7]$$

where $C > 0, \Omega$ is a smooth bounded domain in M, $\text{Area}_g(\partial\Omega)$ is the volume of $\partial\Omega$ for the metric induced by g, and $\text{Vol}_g(\Omega)$ is the volume of Ω with respect to g. Moreover, the constants C and K (for $p = 1$) are the same in the sense that if [6] for $p = 1$ holds with K, then [7] holds with $C = K$, and if [7] holds with C, then [6] for $p = 1$ holds with $K = C$.

The sharp constant for the isoperimetric inequality [7] in Euclidean space is known. When $n = 2$ its value is $C(2) = 1/(4\pi)$ and the sharp isoperimetric inequality is the well-known inequality $L^2 \ge 4\pi A$, where A is the volume of a smooth bounded domain in $\mathbb{R}^2$, and L is the length of its boundary. For arbitrary n, the sharp constant $C(n)$ for the isoperimetric inequality is given by

$$C(n) = \frac{1}{n}\left(\frac{n}{\omega_{n-1}}\right)^{1/n} \quad [8]$$

where ω_{n-1} is the volume of the unit $(n-1)$-sphere. Moreover, still for the Euclidean space, equality holds in the sharp isoperimetric inequality if and only if Ω is a ball. A famous conjecture concerning sharp isoperimetric inequalities, often referred to as the Cartan–Hadamard conjecture, is that the sharp isoperimetric inequality holds on Cartan–Hadamard manifolds. Thanks to works by Croke, Kleiner, and Weil, the conjecture is known to be true in dimensions 2, 3, and 4. From the Bishop–Gromov comparison theorem, we also get that the only complete manifold of non-negative Ricci curvature for which the sharp isoperimetric inequality holds is the Euclidean space itself.

The sharp constants $K = K(n, p)$ for [6] when $p > 1$ have been computed in Euclidean space by Aubin, Rodemich, and Talenti. The extremal functions were also computed, where, by definition, an extremal function is a function which realizes the case of equality in the inequality. We get that

$$K(n,p) = \frac{1}{n}\left(\frac{n(p-1)}{n-p}\right)^{(p-1)/p} \times \left(\frac{\Gamma(n+1)}{\Gamma(n/p)\Gamma(n+1-n/p)\omega_{n-1}}\right)^{1/n} \quad [9]$$

where, as above, Γ is the gamma function. Moreover, u is an extremal function for the sharp inequality in Euclidean space if and only if, up to a scale factor,

$$u(x) = \left(\frac{\mu}{\mu^2 + \frac{|x-a|^{p/(p-1)}}{n(n-2)}}\right)^{(n-p)/p} \quad [10]$$

for some $\mu > 0$, and $a \in \mathbb{R}^n$. When $p = 2$, the functions u in [10] are both the only extremal functions for the sharp Sobolev inequality in Euclidean space, and the only positive solutions of the equation $\Delta u = u^{2^*-1}$ in $\mathbb{R}^n$, where $\Delta = -\sum_i D_i^2$ is the Laplace–Beltrami operator (the usual Laplacian with a minus sign in front of it). Sharp constants are also known for several of the Gagliardo–Nirenberg inequalities in Euclidean space. The sharp constant for the Nash inequality in Euclidean space was computed by Carlen and Loss. If the sharp isoperimetric inequality holds on a complete Riemannian n-manifold, then the sharp inequalities [6] hold for all $1 \leq p < n$.

Sharp Inequalities on Compact Riemannian Manifolds

The study of sharp Sobolev inequalities on compact manifolds if often referred to as the AB program for Sobolev inequalities. For (M, g) a compact Riemannian n-manifold, and $1 \leq p < n$, [5] can be rewritten in two different forms:

$$\left(\int_M |u|^{p^*} dv_g\right)^{1/p^*} \leq A\left(\int_M |\nabla u|^p dv_g\right)^{1/p} + B\left(\int_M |u|^p dv_g\right)^{1/p} \qquad [11]$$

and

$$\left(\int_M |u|^{p^*} dv_g\right)^{p/p^*} \leq A' \int_M |\nabla u|^p dv_g + B' \int_M |u|^p dv_g \qquad [12]$$

where A, B, A', B' are positive constants independent of u. An easy remark is that if [12] holds with constants A' and B', then [11] holds with $A = (A')^{1/p}$ and $B = (B')^{1/p}$. The sharp first (resp. second) constants in [11] and [12] are defined as the lowest possible values for A and A' (resp. for B and B') in [11] and [12]. The sharp first constants are independent of the manifold and are given by $A' = A^p = K(n,p)^p$, where $K(n,p)$ is as in [9]. The sharp second constants depend on the manifold and are given by $B' = B^p = V_g^{-p/n}$, where V_g is the volume of (M, g). A typical question in the AB program is to know whether or not we can take A or B to be the sharp constants in [11] and, similarly, whether or not we can take A' or B' to be the sharp constants in [12]. Another typical question in the AB program is whether or not there are nonzero extremal functions for the saturated form of the sharp inequalities when they are valid. Concerning the B-part of the program, the sharp inequality [11] with $B = V_g^{-1/n}$ is true on any manifold, and constant functions are extremal functions. On the other hand, it can be proved that the stronger [12] with $B' = V_g^{-p/n}$ is always false when $p > 2$, whatever the manifold. Concerning the A-part of the AB-program, Hebey and Vaugon proved that the sharp inequality [12] with $A' = K(n,2)^2$ is true on any manifold. In other words, for any compact Riemannian manifold (M, g) of dimension $n \geq 3$, there exists $B' > 0$ such that, for any $u \in H^{1,2}(M)$,

$$\left(\int_M |u|^{2^*} dv_g\right)^{2/2^*} \leq K(n,2)^2 \int_M |\nabla u|^2 dv_g + B' \int_M |u|^2 dv_g \qquad [13]$$

We then get the saturated form of [13] by taking $B' = B'(g)$ to be the lowest possible B' in [13]. In general, when $p \neq 2$, we can prove that the sharp inequality [11] with $A = K(n,p)$ is true on any manifold, and that there are nonzero extremal functions for the saturated form of the sharp inequality. On the other hand, the stronger [12] with $A' = K(n,p)^p$ when $p > 2$ is false when the curvature is positive, but true when the curvature is negative. The $p = 2$ case in the A-part of the AB program is of importance for its connection with the Yamabe problem. The $p = 1$ case in the A-part of the AB program is of importance for its connection with the isoperimetric inequality. The AB program has also been considered for Gagliardo–Nirenberg inequalities, including the Nash inequality, and Sobolev–Poincaré inequalities on compact manifolds.

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Infinite-Dimensional Hamiltonian Systems

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Introduction

Infinite-dimensional Hamiltonian systems arise in many areas in pure and applied mathematics and in mathematical physics. These are partial differential equations (PDEs) which can be written as evolution equations (dynamical systems) in the form

$$\dot{F} = \{F, H\}$$

where H is the Hamiltonian ("energy") and $\{.,.\}$ is a Poisson bracket on an infinite-dimensional phase space, called Poisson manifold. Unlike finite-dimensional Hamiltonian systems, which are ordinary differential evolution equations on finite-dimensional phase spaces, for which general existence and uniqueness theorems for solutions exist, this is not the case for PDEs. There are no general existence and uniqueness theorems for solutions of infinite-dimensional Hamiltonian systems. These have to be established case by case. This article gives only a broad mathematical framework of infinite-dimensional Hamiltonian systems. Precise definitions are presented and the concept is illustrated through physical examples.

Hamilton's Equations on Poisson Manifolds

A Poisson manifold is a manifold P (in general infinite dimensional) equipped with a bilinear operation $\{.,.\}$, called Poisson bracket, on the space $C^\infty(P)$ of smooth functions on P such that:

1. $(C^\infty(P), \{.,.\})$ is a Lie algebra, that is, $\{.,.\}: C^\infty(P) \times C^\infty(P) \to C^\infty(P)$ is bilinear, skew-symmetric and satisfies the Jacobi identity $\{\{F,G\},H\} + \{\{H,F\},G\} + \{\{G,H\},F\} = 0$ for all $F, G, H \in C^\infty(P)$ and
2. $\{.,.\}$ satisfies the Leibniz rule, that is, $\{.,.\}$ is a derivation in each factor: $\{F \cdot G, H\} = F \cdot \{G, H\} + G \cdot \{F, H\}$, for all $F, G, H \in C^\infty(P)$.

The notion of Poisson manifolds was rediscovered many times under different names, starting with Lie, Dirac, Pauli, and others. The name Poisson manifold was coined by Lichnerowicz.

For any $H \in C^\infty(P)$, the Hamiltonian vector field X_H is defined by

$$X_H(F) = \{F, H\}, \quad F \in C^\infty(P)$$

It follows from (2) that, indeed, X_H defines a derivation on $C^\infty(P)$, hence a vector field on P. Hamilton's equations of motion for a function $F \in C^\infty(P)$ with Hamiltonian H (energy function) are then defined by the flow (integral curves) of the vector field X_H, that is,

$$\dot{F} = X_H(F) = \{F, H\} \qquad [1]$$

where the overdot implies differentiation with respect to time. F is then called a Hamiltonian system on P with energy (Hamiltonian function) H.

Examples of Poisson Manifolds and Hamilton's Equations

Finite-Dimensional Classical Mechanics

For finite-dimensional classical mechanics, we take $P = \mathbb{R}^{2n}$ and coordinates $(q^1, \ldots, q^n, p_1, \ldots, p_n)$ with the standard Poisson bracket for any two functions $F(q^i, p_i), H(q^i, p_i)$ given by

$$\{F, H\} = \sum_{i=1}^{n} \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q^i} - \frac{\partial H}{\partial p_i}\frac{\partial F}{\partial q^i} \qquad [2]$$

Then the classical Hamilton's equations are

$$\begin{aligned} \dot{q}^i &= \{q^i, H\} = \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= \{p_i, H\} = -\frac{\partial H}{\partial q^i} \end{aligned} \qquad [3]$$

$i = 1, \ldots, n$. This finite-dimensional Hamiltonian system is a system of ordinary differential equations for which there are well-known existence and uniqueness theorems, that is, it has locally unique smooth solutions, depending smoothly on the initial conditions.

Example: harmonic oscillator As a concrete example, consider the harmonic oscillator: here $P = \mathbb{R}^2$ and the Hamiltonian (energy) is $H(q,p) = \frac{1}{2}(q^2 + p^2)$. Then Hamilton's equations are

$$\dot{q} = p, \qquad \dot{p} = -q \qquad [4]$$

Infinite-Dimensional Classical Field Theory

Let V be a Banach space and V^* its dual space with respect to a pairing $\langle .,. \rangle : V \times V^* \to \mathbb{R}$ (i.e., $\langle .,. \rangle$ is a symmetric, bilinear, and nondegenerate function). On $P = V \times V^*$, the canonical Poisson

bracket for $F, H \in C^\infty(P)$, $\varphi \in V$, and $\pi \in V^*$ is given by

$$\{F, H\} = \left\langle \frac{\delta F}{\delta \pi}, \frac{\delta H}{\delta \varphi} \right\rangle - \left\langle \frac{\delta H}{\delta \pi}, \frac{\delta F}{\delta \varphi} \right\rangle \qquad [5]$$

where the functional derivatives $\delta F/\delta\pi \in V, \delta F/\delta\varphi \in V^*$ are the "duals" under the pairing $\langle .,. \rangle$ of the partial gradients $D_1 F(\pi) \in V^*, D_2 F(\varphi) \in V^{**} \simeq V$. The corresponding Hamilton's equations are

$$\begin{aligned} \dot{\varphi} &= \{\varphi, H\} = \frac{\delta H}{\delta \pi} \\ \dot{\pi} &= \{\pi, H\} = -\frac{\delta H}{\delta \varphi} \end{aligned} \qquad [6]$$

As a special case in finite dimensions, if $V \simeq \mathbb{R}^n$ so $V^* \simeq \mathbb{R}^n$ and $P = V \times V^* \simeq \mathbb{R}^{2n}$, and the pairing is the standard inner product in $\mathbb{R}^n$, then the Poisson bracket [5] and Hamilton's equations [6] are identical with [2] and [3], respectively.

Example: wave equations As a concrete example, consider the wave equations. Let $V = C^\infty(\mathbb{R}^3)$ and $V^* = \mathrm{Den}(\mathbb{R}^3)$ (densities) and the L^2 pairing $\langle \varphi, \pi \rangle = \int \varphi(x)\pi(x)\,dx$. Take the Hamiltonian to be

$$H(\varphi, \pi) = \int \left(\tfrac{1}{2}\pi^2 + \tfrac{1}{2}|\nabla\varphi|^2 + F(\varphi) \right) dx$$

where F is some function on V. Then Hamilton's equations [6] become

$$\dot{\varphi} = \pi, \quad \dot{\pi} = \nabla^2\varphi - F'(\varphi) \qquad [7]$$

where the prime denotes differentiation with respect to φ, which imply the wave equation

$$\frac{\partial^2 \varphi}{\partial t^2} = \nabla^2\varphi - F'(\varphi) \qquad [8]$$

Different choices of F give different wave equations, for example, for $F = 0$ we get the linear wave equation

$$\frac{\partial^2 \varphi}{\partial t^2} = \nabla^2\varphi$$

for $F = (1/2)m\varphi$, we get the Klein–Gordon equation

$$\nabla^2\varphi - \frac{\partial^2 \varphi}{\partial t^2} = m\varphi$$

So, these wave equations and the Klein–Gordon equation are infinite-dimensional Hamiltonian systems on $P = C^\infty(\mathbb{R}^3) \times \mathrm{Den}\,(\mathbb{R}^3)$.

Cotangent Bundles

The finite-dimensional examples of Poissson brackets [2] and Hamilton's equations [3] and the infinite-dimensional examples [5] and [6] are the local versions of the general case where $P = T^*Q$ is the cotangent bundle (phase space) of a manifold Q (configuration space). If Q in an n-dimensional manifold, then T^*Q is a $2n$-Poisson manifold locally isomorphic to $\mathbb{R}^{2n}$ whose Poisson bracket is locally given by [2] and Hamilton's equations are locally given by [3]. If Q is an infinite-dimensional Banach manifold, then T^*Q is a Poisson manifold locally isomorphic to $V \times V^*$ whose Poisson bracket is given by [5] and Hamilton's equations are locally given by [6].

Symplectic Manifolds

All the examples above are special cases of symplectic manifolds (P, ω). This means that P is equipped with a symplectic structure ω which is a closed $(d\omega = 0)$, (weakly) nondegenerate 2-form on the manifold P. Then, for any $H \in C^\infty(P)$, the corresponding Hamiltonian vector field X_H is defined by $dH = \omega(X_H, .)$ and the canonical Poisson bracket is given by

$$\{F, H\} = \omega(X_F, X_H), \quad F, H \in C^\infty(P) \qquad [9]$$

For example, on $\mathbb{R}^{2n}$ the canonical symplectic structure ω is given by $\omega = \sum_{i=1}^n dp_i \wedge dq^i = d\theta$, where $\theta = \sum_{i=1}^n p_i \wedge dq^i$. The same formula for ω holds locally in T^*Q for any finite-dimensional Q (Darboux's lemma). For the infinite-dimensional example $P = V \times V^*$, the symplectic form ω is given by $\omega((\varphi_1, \pi_1), (\varphi_2, \pi_2)) = \langle \varphi_1, \pi_2 \rangle - \langle \varphi_2, \pi_1 \rangle$. Again, these two formulas for ω are identical if $V = \mathbb{R}^n$.

Remarks

(i) If P is a finite-dimensional symplectic manifold, then P is even dimensional.
(ii) If the Poisson bracket $\{.,.\}$ is nondegenerate, then $\{.,.\}$ comes form a symplectic form ω, that is, $\{.,.\}$ is given by [9].

The Lie–Poisson Bracket

Not all Poisson brackets are of the from given in the above examples [2], [5], and [9], that is, not all Poisson manifolds are symplectic manifolds. An important class of Poisson bracket is the so-called Lie–Poisson bracket. It is defined on the dual of any Lie algebra. Let G be a Lie group with Lie algebra $\mathfrak{g} = T_eG \simeq$ {left-invariant vector fields on G} and let $[.,.]$ denote the Lie bracket (commutator) on $\mathfrak{g}$. Let $\mathfrak{g}^*$ be the dual of a $\mathfrak{g}$ with respect to a pairing $\langle .,. \rangle : \mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$. Then, for any $F, H \in C^\infty(\mathfrak{g}^*)$ and $\mu \in \mathfrak{g}^*$, the Lie–Poisson bracket is defined by

$$\{F, H\}(\mu) = \pm \left\langle \mu, \left[\frac{\delta F}{\delta \mu}, \frac{\delta H}{\delta \mu} \right] \right\rangle \qquad [10]$$

where $\delta F/\delta\mu, \delta H/\delta\mu \in \mathfrak{g}$ are the "duals" of the gradients $DF(\mu), DH(\mu) \in \mathfrak{g}^{**} \simeq \mathfrak{g}$ under the pairing $\langle .,. \rangle$. Note that the Lie–Poisson bracket is degenerate in general, for example, for $G = \mathrm{SO}(3)$ the vector space $\mathfrak{g}^*$ is three dimensional, so the Poisson bracket [10] cannot come from a symplectic structure. This Lie–Poisson bracket can also be obtained in a different way by taking the canonical Poisson bracket on T^*G (locally given by [2] and [5] and then restrict it to the fiber at the identity $T_e^*G = \mathfrak{g}^*$. In this sense, the Lie–Poisson bracket [10] is induced from the canonical Poisson bracket on T^*G. It is induced by the symmetry of left-multiplication, as discussed in the next section.

Example: rigid body A concrete example of the Lie–Poisson bracket is given by the rigid body. Here $G = \mathrm{SO}(3)$ is the configuration space of a free rigid body. Identifying the Lie algebra $(\mathfrak{so}(3), [.,.])$ with $(\mathbb{R}^3, \times)$, where $\times$ is the vector product on $\mathbb{R}^3$ and $\mathfrak{g}^* = \mathfrak{so}(3)^* \simeq \mathbb{R}^3$, the Lie–Poisson bracket translates into

$$\{F, H\}(m) = -m \cdot (\nabla F \times \nabla H) \qquad [11]$$

For any $F \in C^\infty(\mathfrak{so}(3)^*)$, we have

$$\frac{\mathrm{d}F}{\mathrm{d}t}(m) = \nabla F \cdot \dot{m} = \{F, H\}(m)$$
$$= -m \cdot (\nabla F \times \nabla H) = \nabla F \cdot (m \times \nabla H)$$

hence $\dot{m} = m \times \nabla H$. With the Hamiltonian

$$H = \frac{1}{2}\left(\frac{m_1^2}{I_1^2} + \frac{m_2^2}{I_2^2} + \frac{m_3^2}{I_3^2}\right)$$

we get Hamilton's equation as

$$\dot{m}_1 = \frac{I_2 - I_3}{I_2 I_3} m_2 m_3, \qquad \dot{m}_2 = \frac{I_3 - I_1}{I_3 I_1} m_3 m_1$$
$$\dot{m}_3 = \frac{I_1 - I_2}{I_1 I_2} m_1 m_2$$

These are Euler's equations for the free rigid body.

Reduction by Symmetries

The examples discussed so far are all canonical examples of Poisson brackets, defined either on a symplectic manifold (P, ω) or T^*Q, or on the dual of a Lie algebra $\mathfrak{g}^*$. Different, noncanonical Poisson brackets can arise from symmetries. Assume that a Lie group G is acting in a Hamiltonian way on the Poisson manifold $(P, \{..\})$. This means that we have a smooth map $\varphi : G \times P \to P : \varphi(g, p) = g \cdot p$ such that the induced maps $\varphi_g = \varphi(g, .) : P \to P$ are canonical transformations, for each $g \in G$. In terms of Poisson manifolds, a canonical transformation is a smooth map that preserves the Poisson bracket. So, the action of G on P is a Hamiltonian action if $\varphi_g^*\{F, H\} = \{\varphi_g^* F, \varphi_g^* H\}$ for all $F, H \in C^\infty(P)$, $g \in G$. For any $\xi \in \mathfrak{g}$, the canonical transformations $\varphi_{\exp(t\xi)}$ generate a Hamiltonian vector field ξ_F on P and a momentum map $J : P \to \mathfrak{g}^*$ given by $J(x)(\xi) = F(x)$, which is Ad^* equivariant.

If a Hamiltonian system X_H is invariant under a Lie group action, that is, $H(\varphi_g(x)) = H(x)$, then we obtain a reduced Hamiltonian system on a reduced phace space (reduced Poisson manifold). We recall the Marsden–Weinstein reduction theorem:

Reduction Theorem *For a Hamiltonian action of a Lie group G on a Poisson manifold $(P, \{.,.\})$, there is an equivariant momentum map $J : P \to \mathfrak{g}^*$, and for every regular $\mu \in \mathfrak{g}^*$ the reduced phase space $P_\mu \equiv J^{-1}(\mu)/G_\mu$ carries an induced Poisson structure $\{.,.\}_\mu$, (G_μ the isotropy group). Any G-invariant Hamiltonian H on P defines a Hamiltonian H_μ on the reduced phase space P_μ and the integral curves of the vector field X_H project onto integral curves of the induced vector field $\hat{X}_{H_\mu}$ on the reduced space P_μ.*

Example: rigid body The rigid body discussed above can be viewed as an example of this reduction theorem. If $P = T^*G$ and G is acting on T^*G by the cotangent lift of the left-translation $l_g : G \to G, l_g(h) = gh$, then the momentum map $J : T^*G \to \mathfrak{g}^*$ is given by $J(\alpha_g) = T_e^* R_g(\alpha_g)$ and the reduced phase space $(T^*G)_\mu = J^{-1}(\mu)/G_\mu$ is isomorphic to the coadjoint orbit $\mathcal{O}_\mu$ through $\mu \in \mathfrak{g}^*$. Each coadjoint orbit $\mathcal{O}_\mu$ carries a natural symplectic structure ω_μ and in this case, the reduced Lie–Poisson bracket $\{.,.\}_\mu$ on the coadjoint orbit $\mathcal{O}_\mu$ is induced by the symplectic form ω_μ on $\mathcal{O}_\mu$ as in [9]. Furthermore, $T^*G/G \simeq \mathfrak{g}^*$, and the induced Poisson bracket $\{.,.\}_\mu$ on $\mathcal{O}_\mu$ is identical with the Lie–Poisson bracket restricted to the coadjoint orbit $\mathcal{O}_\mu \subset \mathfrak{g}^*$. For the rigid body this construction is applied to $G = \mathrm{SO}(3)$.

We now discuss some infinite-dimensional examples of reduced Hamiltonian systems.

Infinite-Dimensional Lie Groups

A general theory of infinite-dimensional Lie groups is hardly developed. Even Bourbaki only develops a theory of infinite-dimensional manifolds, but all of the important theorems about Lie groups are stated for finite-dimensional ones.

An infinite-dimensional Lie group $\mathcal{G}$ is a group and an infinite-dimensional manifold with smooth group operations

$$m : \mathcal{G} \times \mathcal{G} \to \mathcal{G}, \quad m(g,h) = g \cdot h, \qquad C^\infty \qquad [12]$$

$$i : \mathcal{G} \to \mathcal{G}, \quad i(g) = g^{-1}, \qquad C^\infty \qquad [13]$$

Such a Lie group $\mathcal{G}$ is locally diffeomorphic to an infinite-dimensional vector space. This can be a Banach space whose topology is given by a norm $\|\cdot\|$, a Hilbert space whose topology is given by an inner product $\langle .,. \rangle$, or a Frechet space whose topology is given by a metric but not by a norm. Depending on the choice of the topology on $\mathcal{G}$, the Banach, Hilbert, or Frechet Lie groups, respectively, can be treated.

The Lie algebra $\mathfrak{g}$ of $\mathcal{G}$ is defined as $\mathfrak{g} = \{\text{left-invariant vector fields on } \mathcal{G}\} \simeq T_e\mathcal{G}$, where the isomorphism is given (as in finite dimensions) by

$$\xi \in T_e\mathcal{G} \mapsto X^\xi(g) = T_eL_g(\xi) \qquad [14]$$

and the Lie bracket on $\mathfrak{g}$ is induced by the Lie bracket of left-invariant vector fields $[\xi,\eta] = [X^\xi, X^\eta](e)$, $\xi, \eta \in \mathfrak{g}$.

These definitions in infinite dimensions are identical with the definitions in finite dimensions. The big difference although is that infinite-dimensional manifolds, hence Lie groups, are not locally compact. For Frechet Lie groups, one has the additional nontrivial difficulty of defining the differentiability of functions defined on a Frechet space. Hence, the very definition of a Frechet manifold is not canonical. This problem does not arise for Banach and Hilbert Lie groups; the differential calculus extends in a straightforward manner from $\mathbb{R}^n$ to Banach and Hilbert spaces, but not to Frechet spaces.

Finite- versus Infinite-Dimensional Lie Groups

The lack of local compactness of infinite-dimensional Lie groups causes some deficiencies of the Lie theory in infinite dimensions. Some classical results in finite dimensions are summarized below, which are not true in general in infinite dimensions:

1. The exponential map $exp : \mathfrak{g} \to G$ is defined as follows: To each $\xi \in \mathfrak{g}$ we assign the corresponding left-invariant vector field X^ξ defined by [14]. We take the flow $\varphi^\xi(t)$ of X^ξ and define $exp(\xi) = \varphi^\xi(1)$. The exponential map is a local diffeomorphism from a neighborhood of zero in $\mathfrak{g}$ onto a neighborhood of the identity in G; hence, exp defines canonical coordinates on the Lie group G. This is not true in infinite dimensions.
2. If $f_1, f_2 : G_1 \to G_2$ are smooth Lie group homomorphisms (i.e., $f_i(g \cdot h) = f_i(g) \cdot f_i(h), i = 1, 2$) with $T_ef_1 = T_ef_2$, then locally $f_1 = f_2$. This is not true in infinite dimensions.
3. If H is a closed subgroup of G, then H is a Lie subgroup of G. This is not true in infinite dimensions.
4. For any finite-dimensional Lie algebra $\mathfrak{g}$, there exists a connected Lie group G whose Lie algebra is $\mathfrak{g}$, that is, such that $\mathfrak{g} \simeq T_eG$. This is not true in infinite dimensions.

Some classical finite-dimensional examples of Lie groups are the matrix groups $GL(n)$, $SL(n)$, $O(n)$, $SO(n)$, $U(n)$, $SU(n)$, $Sp(n)$ with smooth group operations given by matrix multiplication and matrix inversion.

Examples of Infinite-Dimensional Lie Groups

Abelian Gauge Group $\mathcal{G} = (C^\infty(M), +)$

Let M be a finite-dimensional manifold and let $\mathcal{G} = C^\infty(M)$. With group operation being addition, that is, $m(f,g) = f + g$, $i(f) = -f$, $e = 0$. $\mathcal{G}$ is an abelian C^∞ Frechet Lie group with Lie algebra $\mathfrak{g} = T_eC^\infty(M) \simeq C^\infty(M)$, with trivial bracket $[\xi,\eta] = 0$, and $exp = \text{id}$. If one completes these spaces in the C^k-norm, $k < \infty$ then $\mathcal{G}^k$ is a Banach Lie group, and if the H^s-Sobolev norm is used with $s > (1/2)\dim M$ then $\mathcal{G}^s$ is a Hilbert Lie group.

Application of $\mathcal{G} = (C^\infty(M), +)$ to Maxwell's equations Let E, B be the electric and magnetic fields on $\mathbb{R}^3$; then Maxwell's equations for a charge density ρ are:

$$\dot{E} = \text{curl}\, B, \qquad \dot{B} = -\text{curl}\, E \qquad [15]$$

$$\text{div}\, B = 0, \qquad \text{div}\, E = \rho \qquad [16]$$

Let A be the magnetic potential such that $B = -\text{curl}\, A$. As configuration space, we take $V = \text{Vec}(\mathbb{R}^3)$, vector fields (potentials) on $\mathbb{R}^3$, so $A \in V$, and as phase space, we have $P = T^*V \simeq V \times V^* \ni (A, E)$, with the standard L^2 pairing $\langle A, E\rangle = \int A(x)E(x)\,dx$, and canonical Poisson bracket given by [5], which becomes

$$\{F,H\}(A,E) = \int \left(\frac{\delta F}{\delta A}\frac{\delta H}{\delta E} - \frac{\delta H}{\delta A}\frac{\delta F}{\delta E} \right) dx \qquad [17]$$

As Hamiltonian, we take the total electromagnetic energy

$$H(A, E) = \frac{1}{2}\int (|\text{curl } A|^2 + |E|^2)\, dx$$

Then Hamilton's equations in the canonical variables A and E are

$$\dot{A} = \frac{\delta H}{\delta E} = E \Rightarrow \dot{B} = -\text{curl}\, E$$

and

$$\dot{E} = -\frac{\delta H}{\delta A} = -\text{curl}\,\text{curl}\, A = \text{curl}\, B$$

So the first two equations of Maxwell's equations [15] are Hamilton's equations, the third one is obtained automatically from the potential $\text{div} B = -\text{div}\,\text{curl} A = 0$ and the fourth equation, $\text{div} E = \rho$, is obtained through the following symmetry (gauge invariance): the Lie group $\mathcal{G} = (C^\infty(\mathbb{R}^3), +)$ acts on V by $\varphi \cdot A = A + \nabla\varphi, \varphi \in \mathcal{G}, A \in V$. The lifted action to $V \times V^*$ becomes $\varphi \cdot (A, E) = (A + \nabla\varphi, E)$, and has the momentum map $J : V \times V^* \to \mathfrak{g}^* \simeq$ {charge densities}

$$J(A, E) = \text{div}\, E \qquad [18]$$

With $\mathfrak{g} = C^\infty(\mathbb{R}^3)$ and $\mathfrak{g}^* = \text{Den}(\mathbb{R}^3)$, we identify the elements of $\mathfrak{g}^*$ with charge densities. The Hamiltonian H is $\mathcal{G}$ invariant, that is, $H(\varphi \cdot (A, E)) = H(A + \nabla\varphi, E) = H(A, E)$. Then the reduced phase space for $\rho \in \mathfrak{g}^*$ is

$$(V \times V^*)_\rho = J^{-1}(\rho)/G = \{(E, B) | \text{div} E = \rho,\ \text{div} B = 0\}$$

and the reduced Hamiltonian is

$$H_\rho(E, B) = \frac{1}{2}\int (|E|^2 + |B|^2)\, dx \qquad [19]$$

The reduced Poisson bracket becomes, for any functions F, H on $(V \times V^*)_\rho$,

$$\{F, H\}_\rho(E, B) = \int \left(\frac{\delta F}{\delta E} \cdot \text{curl}\, \frac{\delta H}{\delta B} - \frac{\delta H}{\delta E} \cdot \text{curl}\, \frac{\delta F}{\delta B}\right) dx \qquad [20]$$

and a straightforward computation shows that

$$\dot{F} = \{F, H_\rho\}_\rho \Leftrightarrow \begin{cases} \dot{E} = \text{curl}\, B, & \dot{B} = -\text{curl}\, E \\ \text{div}\, B = 0, & \text{div}\, E = \rho \end{cases} \qquad [21]$$

So, Maxwell's equations [15], [16] form an infinite-dimensional Hamiltonian system on this reduced phase space with respect to the reduced Poisson bracket.

Abelian Gauge Group $\mathcal{G} = (C^\infty(M, \mathbb{R} - \{0\}), \cdot)$

Let M be a finite-dimensional manifold and let $\mathcal{G} = C^\infty(M, \mathbb{R} - \{0\})$, the group operation being the multiplication, that is, $m(f, g) = f \cdot g$, $i(f) = f^{-1}$, $e = 1$. For $k < \infty$, $C^k(M, \mathbb{R} - \{0\})$ is open in $C^\infty(M, \mathbb{R})$, and if M is compact then $C^k(M, \mathbb{R} - \{0\})$ is a Banach Lie group. If $s > (1/2)\dim M$ then $H^s(M, \mathbb{R} - \{0\})$ is closed under multiplication, and if M is compact then $H^s(M, \mathbb{R} - \{0\})$ is a Hilbert Lie group.

Nonabelian Gauge Groups $\mathcal{G} = (C^k(M, G), \cdot)$

The abelian example can be generalized by replacing $\mathbb{R} - \{0\}$ with any finite-dimensional (nonabelian) Lie group G. Let $\mathcal{G} = C^k(M, G)$ with pointwise group operations $m(f, g)(x) = f(x) \cdot g(x), x \in M$ and $i(f)(x) = (f(x))^{-1}$, where "$\cdot$" and "$(\,.\,)^{-1}$" are the operations in G. If $k < \infty$ then $C^k(M, G)$ is a Banach Lie group. Let g denote the Lie algebra of G, then the Lie algebra of $\mathcal{G} = C^k(M, G)$ is $\mathfrak{g} = C^k(M, g)$, with pointwise Lie bracket $[\xi, \eta](x) = [\xi(x), \eta(x)], x \in M$, the latter bracket being the Lie bracket in g. The exponential map $exp : g \to G$ defines the exponential map $EXP : \mathfrak{g} = C^k(M, g) \to \mathcal{G} = C^k(M, G)$, $EXP(\xi) = exp \circ \xi$, which is a local diffeomorphism. The same holds for $H^s(M, G)$ if $s > (1/2)\dim M$.

Applications of these infinite-dimensional Lie groups are in gauge theories and quantum field theory, where they appear as groups of gauge transformations.

Loop Groups $\mathcal{G} = C^k(S^1, G)$

As a special case of the example above, we take $M = S^1$, the circle. Then $\mathcal{G} = C^k(S^1, G) = \mathcal{L}^k(G)$ is called a loop group and $\mathfrak{g} = C^k(S^1, g) = l^k(g)$ its loop algebra. They find applications in the theory of affine Lie algebras, Kac–Moody Lie algebras (central extensions), completely integrable systems, soliton equations (Toda, Korteweg–de Vries (KdV), Kadomtsev–Petviashvili (KP)), quantum field theory. Central extensions of Loop algebras are examples of infinite-dimensional Lie algebras which need not have a corresponding Lie group.

Diffeomorphism Groups

Among the most important "classical" infinite-dimensional Lie groups are the diffeomorphism groups of manifolds. Their differential structure is not the one of a Banch Lie group as defined above. Nevertheless, they have important applications.

Let M be a compact manifold (the noncompact case is technically much more complicated but similar results are true) and let $\mathcal{G} = \text{Diff}^\infty(M)$ be the group of all smooth diffeomorphisms on M,

group operation being the composition, that is, $m(f,g) = f \circ g$, $i(f) = f^{-1}$, $e = \mathrm{id}_M$. For C^∞ diffeomorphisms, $\mathrm{Diff}^\infty(M)$ is a Frechet manifold and there are nontrivial problems with the notion of smooth maps between Frechet spaces. There is no canonical extension of the differential calculus from Banach spaces (same as for $\mathbb{R}^n$) to Frechet spaces. One possibility is to generalize the notion of differentiability. For example, if we use the so-called C^∞_Γ differentiability, then $\mathcal{G} = \mathrm{Diff}^\infty(M)$ becomes a C^∞_Γ Lie group with C^∞_Γ differentiable group operations. These notions of differentiability are difficult to apply to concrete examples. Another possibility is to complete $\mathrm{Diff}^\infty(M)$ in the Banach C^k-norm, $0 \leq k < \infty$, or in the Sobolev H^s-norm, $s > (1/2)\dim M$; $\mathrm{Diff}^k(M)$ and $\mathrm{Diff}^s(M)$ become, in this case, Banach and Hilbert manifolds, respectively. Then we consider the inverse limits of these Banach and Hilbert Lie groups, respectively:

$$\mathrm{Diff}^\infty(M) = \lim_{\leftarrow} \mathrm{Diff}^k(M) \qquad [22]$$

becomes the so-called inverse limit of Banach (ILB) Lie group, or with the Sobolev topologies

$$\mathrm{Diff}^\infty(M) = \lim_{\leftarrow} \mathrm{Diff}^s(M) \qquad [23]$$

becomes the so-called inverse limit of Hilbert (ILH) Lie group. Nevertheless, the group operations are not smooth, but have the following differentiability properties. If the diffeomorphism group is equipped with the Sobolev H^s-topology, then $\mathrm{Diff}^s(M)$ becomes a C^∞ Hilbert manifold if $s > (1/2)\dim M$ and the group multiplication

$$m : \mathrm{Diff}^{s+k}(M) \times \mathrm{Diff}^s(M) \to \mathrm{Diff}^s(M) \qquad [24]$$

is C^k differentiable; hence, for $k = 0$, m is only continuous on $\mathrm{Diff}^s(M)$. The inversion

$$i : \mathrm{Diff}^{s+k}(M) \to \mathrm{Diff}^s(M) \qquad [25]$$

is C^k differentiable; hence, for $k = 0$, i is only continuous on $\mathrm{Diff}^s(M)$. The same differentiability properties of m and i hold in the C^k topology. This situation leads to the notion of nested Lie groups.

The Lie algebra of $\mathrm{Diff}^\infty(M)$ is given by $\mathfrak{g} = T_e\mathrm{Diff}^\infty(M) \simeq \mathrm{Vec}^\infty(M)$, the space of smooth vector fields on M. Note that the space $\mathrm{Vec}(M)$ of all vector fields is a Lie algebra only for C^∞ vector fields, but not for C^k or H^s vector fields if $k < \infty$, $s < \infty$, because one loses derivatives by taking brackets.

The exponential map on the diffeomorphism group is given as follows: for any vector field $X \in \mathrm{Vec}^\infty(M)$ take its flow $\varphi_t \in \mathrm{Diff}^\infty(M)$, then define $EXP : \mathrm{Vec}^\infty(M) \to \mathrm{Diff}^\infty(M) : X \mapsto \varphi_1$, the flow at time $t = 1$. The exponential map EXP is not a local diffeomorphism; it is not even locally surjective.

Applications of $\mathrm{Diff}^\infty(M)$ occur in general relativity, where the diffeomorphism group plays the role of a symmetry group of coordinate transformations. Let (M, g) be a Lorentz 4-manifold. Then the vacuum Einstein's field equations are

$$\mathrm{Ric}(g) = 0$$

These are invariant under coordinate transformations, that is, under the action of $\mathrm{Diff}^\infty(M)$. Moreover, Einstein's field equations form a Hamiltonian system on the space $P = \{\text{metrics on } M\}/\mathrm{Diff}^\infty(M)$.

Subgroups of $\mathrm{Diff}^\infty(M)$

Several subgroups of $\mathrm{Diff}^\infty(M)$ have important applications.

Group of volume-preserving diffeomorphisms Let μ be a volume on M and $\mathcal{G} = \mathrm{Diff}^\infty_\mu(M) = \{f \in \mathrm{Diff}^\infty(M) \mid f^*\mu = \mu\}$ the group of volume-preserving diffeomorphisms. $\mathrm{Diff}^\infty_\mu(M)$ is a closed subgroup of $\mathrm{Diff}^\infty(M)$ with Lie algebra $\mathfrak{g} = \mathrm{Vec}^\infty_\mu(M) = \{X \in \mathrm{Vec}^\infty(M) \mid \mathrm{div}_\mu X = 0\}$ the space of divergence free vector fields on M. $\mathrm{Vec}^\infty_\mu(M)$ is a Lie subalgebra of $\mathrm{Vec}^\infty(M)$.

Remark: We can neither apply the finite-dimensional theorem that if $\mathrm{Vec}^\infty_\mu(M)$ is Lie algebra then there exists a Lie group whose Lie algebra it is; nor that if $\mathrm{Diff}^\infty_\mu(M) \subset \mathrm{Diff}(M)$ is a closed subgroup then it is a Lie subgroup.

Applications of $\mathrm{Diff}^\infty_\mu(M)$ occur, for example, in fluid dynamics. Euler's equations for an incompressible fluid,

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p, \qquad \mathrm{div}\, u = 0 \qquad [26]$$

are equivalent to the equations of geodesics on $\mathrm{Diff}^\infty_\mu(M)$.

Symplectomorphism group Let ω be a symplectic 2-from on M and $\mathcal{G} = \mathrm{Diff}^\infty_\omega(M) = \{f \in \mathrm{Diff}^\infty(M) \mid f^*\omega = \omega\}$ the group of canonical transformations (or symplectomorphisms). $\mathrm{Diff}^\infty_\omega(M)$ is a closed subgroup of $\mathrm{Diff}^\infty(M)$ with Lie algebra $\mathfrak{g} = \mathrm{Vec}^\infty_\omega(M) = \{X \in \mathrm{Vec}^\infty(M) \mid L_X\omega = 0\}$ the space of locally Hamiltonian vector fields on M. $\mathrm{Vec}^\infty_\omega(M)$ is a Lie subalgebra of $\mathrm{Vec}^\infty(M)$.

Applications of symplectomorphism groups occur, for example, in plasma physics. Maxwell–Vlasov's

equations for a plasma density $f(x, v, t)$ generating the electric and magnetic fields E and B are

$$\begin{aligned} &\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + (E + v \times B)\frac{\partial f}{\partial v} = 0 \\ &\frac{\partial B}{\partial t} = -\mathrm{curl}\, E, \qquad \frac{\partial E}{\partial t} = \mathrm{curl}\, B - J_f \\ &\mathrm{div}\, E = \rho_f, \qquad \mathrm{div}\, B = 0 \end{aligned} \qquad [27]$$

where J_f and ρ_f are the current and charge densities, respectively. This coupled nonlinear system of evolution equations is an infinite-dimensional Hamiltonian system of the form $\dot{F} = \{F, H\}_{\rho_f}$ on the reduced phace space

$$\mathcal{MV} = (T^*\mathrm{Diff}^\infty_\omega(\mathbb{R}^6) \times T^*V)/C^\infty(\mathbb{R}^6) \qquad [28]$$

(V is the same space as in the example of Maxwell's equations) with respect to the following reduced Poisson bracket, which is induced via gauge symmetry from the canonical Poisson bracket on $T^*\mathrm{Diff}^\infty_\omega(\mathbb{R}^6) \times T^*V$:

$$\begin{aligned} &\{F, G\}_{\rho_f}(f, E, B) \\ &= \int f\left\{\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right\}\mathrm{d}x\,\mathrm{d}v \\ &+ \int\left(\frac{\delta F}{\delta E}\cdot \mathrm{curl}\frac{\delta G}{\delta B} - \frac{\delta G}{\delta E}\cdot \mathrm{curl}\frac{\delta F}{\delta B}\right)\mathrm{d}x\,\mathrm{d}v \\ &+ \int\left(\frac{\delta F}{\delta E}\cdot\frac{\partial f}{\partial v}\frac{\delta G}{\delta f} - \frac{\delta G}{\delta E}\cdot\frac{\partial f}{\partial v}\frac{\delta F}{\delta f}\right)\mathrm{d}x\,\mathrm{d}v \\ &+ \int fB\cdot\left(\frac{\partial}{\partial v}\frac{\delta F}{\delta f} \times \frac{\partial}{\partial v}\frac{\delta G}{\delta f}\right)\mathrm{d}x\,\mathrm{d}v \end{aligned} \qquad [29]$$

and with Hamiltonian

$$\begin{aligned} H(f, E, B) &= \frac{1}{2}\int v^2 f(x, v, t)\mathrm{d}v \\ &+ \frac{1}{2}\int (|E|^2 + |B|^2)\mathrm{d}x \end{aligned} \qquad [30]$$

More complicated plasma models are formulated as Hamiltonian systems. For example, for the two-fluid model the phase space is constituted by coadjoint orbits of the semidirect product ($\ltimes$) of the group $\mathcal{G} = \mathrm{Diff}^\infty(\mathbb{R}^6) \ltimes (C^\infty(\mathbb{R}^6) \times C^\infty(\mathbb{R}^6))$. For the MHD model: $\mathcal{G} = \mathrm{Diff}^\infty(\mathbb{R}^6) \ltimes (C^\infty(\mathbb{R}^6) \times \Omega^2(\mathbb{R}^3))$.

The KdV Equation and Fourier Integral Operators

There are many known examples of PDEs which are infinite-dimensional Hamiltonian systems, such as the Benjamin–Ono, Boussinesq, Harry Dym, KdV, and KP equations and others. In many cases, the Poisson structures and Hamiltonians are given *ad hoc* on a formal level. This is illustrated here with the KdV equation, where at least one of the three known Hamiltonian structures is well understood.

The KdV equation

$$u_t + 6uu_x + u_{xxx} = 0 \qquad [31]$$

is an infinite-dimensional Hamiltonian system with the Lie group of invertible Fourier integral operators being a symmetry group. Gardner found that with the bracket

$$\{F, G\} = \int_0^{2\pi} \frac{\delta F}{\delta u}\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\mathrm{d}x \qquad [32]$$

and Hamiltonian

$$H(u) = \int_0^{2\pi} (u^3 + \tfrac{1}{2}u_x^3)\mathrm{d}x \qquad [33]$$

u satisfies the KdV equation [31] if and only if

$$\dot{u} = \{u, H\}$$

An important question concerns the origin of the Poisson bracket [32] and Hamiltonian [33]. It was shown earlier that this bracket is the Lie–Poisson bracket on a coadjoint orbit of Lie group $\mathcal{G} = \mathrm{FIO}$, the group of invertible Fourier integral operators on the circle S^1. The latter is discussed briefly in the following.

A Fourier integral operator on a compact manifold M is an operator

$$A : C^\infty(M) \to C^\infty(M) \qquad [34]$$

locally given by

$$A(u)(x) = (2\pi)^{-n}\iint e^{i\varphi(x,y,\xi)}a(x, \xi)u(y)\mathrm{d}y\,\mathrm{d}\xi \qquad [35]$$

where $\varphi(x, y, \xi)$ is a phase function with certain properties and the symbol $a(x, \xi)$ belongs to a certain symbol class. A pseudodifferential operator is a special kind of Fourier integral operators, locally of the form

$$P(u)(x) = (2\pi)^{-n}\iint e^{i(x-y)\cdot\xi}p(x, \xi)u(y)\mathrm{d}y\,\mathrm{d}\xi \qquad [36]$$

Denote by FIO and ΨDO the groups under composition (operator product) of invertible Fourier integral operators and invertible pseudodifferential operators on M, respectively. Then we have the following results.

Both groups ΨDO and FIO are smooth infinite-dimensional ILH Lie groups. The smoothness properties of the group operations (operator multiplication and inversion) are similar to the case of diffeomorphism groups [24] and [25]. The Lie algebra of both ILH Lie groups ΨDO and FIO is the Lie algebra of all pseudodifferential operators under the commutator bracket. Moreover, FIO is a smooth infinite-dimensional principal fiber bundle

over the diffeomorphism group of canonical transformations $\mathrm{Diff}^{\infty}_{\omega}(T^*M - \{0\})$ with structure group (gauge group) ΨDO.

For the KdV equation, we take the special case where $M = S^1$. Then the Gardner bracket [32] is the Lie–Poisson bracket on the coadjoint orbit of FIO through the Schrödinger operator $P \in \Psi\mathrm{DO}$. Complete integrability of the KdV equation follows from the infinite system of conserved integrals in involution given by $H_k = \mathrm{tr}(P^k)$; in particular, the Hamiltonian [33] equals $H = H_2$.

See also: Bi-Hamiltonian Methods in Soliton Theory; Functional Integration in Quantum Physics; Hamiltonian Fluid Dynamics; Hamiltonian Systems: Obstructions to Integrability; Korteweg–de Vries Equation and Other Modulation Equations; Symmetries and Conservation Laws.

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Instantons: Topological Aspects

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Introduction

Let X be a closed (connected, compact without boundary) smooth manifold of dimension 4, provided with a Riemannian metric denoted by g. Let Ω^p_X denote space of smooth p-forms on X, that is, the sections of $\wedge^p TX$. The Hodge operator acting on p-forms,

$$* : \Omega^p_X \to \Omega^{4-p}_X$$

satisfies $*^2 = (-1)^p$. In particular, $*$ splits Ω^2_X into two subspaces $\Omega^{2,\pm}_X$ with eigenvalues ± 1:

$$\Omega^2_X = \Omega^{2,+}_X \oplus \Omega^{2,-}_X \qquad [1]$$

Note also that this decomposition is an orthogonal one, with respect to the inner product:

$$\langle \omega_1, \omega_2 \rangle = \int_X \omega_1 \wedge *\omega_2$$

A 2-form ω is said to be self-dual if $*\omega = \omega$ and it is said to be anti-self-dual if $*\omega = -\omega$. Any 2-form ω can be written as the sum

$$\omega = \omega^+ + \omega^-$$

of its self-dual ω^+ and anti-self-dual ω^- components.

Now let E be a complex vector bundle over X as above, provided with a connection ∇, regarded as a $\mathbb{C}$-linear operator

$$\nabla : \Gamma(E) \to \Gamma(E) \otimes \Omega^1_X$$

satisfying the Leibnitz rule:

$$\nabla(f\sigma) = f\nabla\sigma + \sigma \otimes \mathrm{d}f$$

for all $f \in C^\infty(X)$ and $\sigma \in \Gamma(E)$. Its curvature $F_\nabla = \nabla \circ \nabla$ is a 2-form with values in End(E), that is, $F_\nabla \in \Gamma(\mathrm{End}(E)) \otimes \Omega^2_X$, satisfying the Bianchi identity $\nabla F_\nabla = 0$.

The Yang–Mills equation is

$$\nabla * F_\nabla = 0 \qquad [2]$$

It is a second-order nonlinear equation on the connection ∇. It amounts to a nonabelian generalization of Maxwell equations, to which it reduces when E is a line bundle; the four components of ∇ are interpreted as the electric and magnetic potentials.

An instanton on E is a smooth connection ∇ whose curvature F_∇ is anti-self-dual as a 2-form, that is, it satisfies:

$$F^+_\nabla = 0, \quad \text{that is,} \quad * F_\nabla = -F_\nabla \qquad [3]$$

The instanton equation is still nonlinear (it is linear only if E is a line bundle), but it is only first-order on the connection.

Note that if F_∇ is either self-dual or anti-self-dual as a 2-form, then the Yang–Mills equation is automatically satisfied:

$$*F_\nabla = \pm F_\nabla \Rightarrow \nabla * F_\nabla = \pm \nabla F_\nabla = 0$$

by the Bianchi identity. In other words, instantons are particular solutions of the Yang–Mills equation. Furthermore, while the Yang–Mills equation [2] makes sense over any Riemannian manifold, the instanton equation [3] is well defined only in dimension 4.

A gauge transformation is a bundle automorphism $g: E \to E$ covering the identity. The set of all gauge transformations of a given bundle $E \to X$ forms a group through composition, called the gauge group and denoted by $\mathcal{G}(E)$. The gauge group acts on the set of all smooth connections on E by conjugation:

$$g \cdot \nabla = g^{-1} \nabla g$$

It is then easy to see that [3] is a gauge-invariant condition, since $F_{g\cdot\nabla} = g^{-1} F_\nabla g$. The anti-self-duality equation [3] is also conformally invariant: a conformal change in the metric does not change the decomposition [1], so it preserves self-dual and anti-self-dual 2-forms.

The topological charge k of the instanton ∇ is defined by the integral

$$\begin{aligned} k &= -\frac{1}{8\pi^2} \int_X \mathrm{tr}(F_\nabla \wedge F_\nabla) \\ &= c_2(E) - \frac{1}{2} c_1(E)^2 \end{aligned} \qquad [4]$$

where the second equality follows from Chern–Weil theory.

If X is a smooth, noncompact, complete Riemannian manifold, an instanton on X is an anti-self-dual connection for which the integral [4] converges. Note that, in this case, k as above need not be an integer; however, it is always expected to be quantized, that is, always a multiple of some fixed (rational) number which depends only on the base manifold X.

Summary This note is organized as follows. After revisiting the variational approach to the anti-self-duality equation [3], we study instantons over the simplest possible Riemannian 4-manifold, $\mathbb{R}^4$ with the flat Euclidean metric. In the subsequent sections, we present 't Hooft's explicit solutions, the ADHM construction, and its dimensional reductions to $\mathbb{R}^3, \mathbb{R}^2$ and $\mathbb{R}$. We conclude by explaining the construction of the central object of study in gauge theory, the instanton moduli spaces.

Variational Aspects of Yang–Mills Equation

Given a fixed smooth vector bundle $E \to X$, let $\mathcal{A}(E)$ be the set of all (smooth) connections on E. The Yang–Mills functional is defined by

$$\begin{aligned} &\mathrm{YM} : \mathcal{A}(E) \to \mathbb{R} \\ &\mathrm{YM}(\nabla) = \|F_\nabla\|^2_{L^2} = \int_M \mathrm{tr}(F_\nabla \wedge *F_\nabla) \end{aligned} \qquad [5]$$

The Euler–Lagrange equation for this functional is exactly the Yang–Mills equation [2]. In particular, self-dual and anti-self-dual connections yield critical points of the Yang–Mills functional.

Splitting the curvature into its self-dual and anti-self-dual parts, we have

$$\mathrm{YM}(\nabla) = \|F^+_\nabla\|^2_{L^2} + \|F^-_\nabla\|^2_{L^2}$$

It is then easy to see that every anti-self-dual connection ∇ is an absolute minimum for the Yang–Mills functional, and that $\mathrm{YM}(\nabla)$ coincides with the topological charge [4] of the instanton ∇ times $8\pi^2$.

One can construct, for various 4-manifolds but most interestingly for $X = S^4$, solutions of the Yang–Mills equations which are neither self-dual nor anti-self-dual. Such solutions do not minimize [5]. Indeed, at least for gauge group SU(2) or SU(3), it can be shown that there are no other local minima: any critical point which is neither self-dual nor anti-self-dual is unstable and must be a "saddle point" (Bourguignon and Lawson Jr. 1981).

Instantons on Euclidean Space

Let $X = \mathbb{R}^4$ with the flat Euclidean metric, and consider a Hermitian vector bundle $E \to \mathbb{R}^4$. Any connection ∇ on E is of the form $d + A$, where d denotes the usual de Rham operator and $A \in \Gamma(\mathrm{End}(E)) \otimes \Omega^1_{\mathbb{R}^4}$ is a 1-form with values in the endomorphisms of E; this can be written as follows:

$$A = \sum_{k=1}^{4} A_k \, \mathrm{d}x^k, \quad A_k : \mathbb{R}^4 \to \mathfrak{u}(r)$$

In the Euclidean coordinates x_1, x_2, x_3, x_4, the anti-self-duality equation [3] is given by

$$F_{12} = F_{34}, \quad F_{13} = -F_{24}, \quad F_{14} = F_{23}$$

where

$$F_{ij} = \frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} + [A_i, A_j]$$

The simplest explicit solution is the charge-1 SU(2) instanton on $\mathbb{R}^4$. The connection 1-form is given by

$$A_0 = \frac{1}{1+|x|^2} \cdot \mathrm{Im}(q\,\mathrm{d}\bar{q}) \qquad [6]$$

where q is the quaternion $q = x_1 + x_2\boldsymbol{i} + x_3\boldsymbol{j} + x_4\boldsymbol{k}$, while Im denotes the imaginary part of the product quaternion; we are regarding $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$ as a basis of the Lie algebra $\mathfrak{su}(2)$; from this, one can compute the curvature:

$$F_{A_0} = \left(\frac{1}{1+|x|^2}\right)^2 \cdot \mathrm{Im}(\mathrm{d}q \wedge \mathrm{d}\bar{q}) \qquad [7]$$

We see that the action density function

$$|F_{A_0}|^2 = \left(\frac{1}{1+|x|^2}\right)^2$$

has a bell-shaped profile centered at the origin and decays like r^{-4}.

Let $t_{\lambda,y}: \mathbb{R}^4 \to \mathbb{R}^4$ be the isometry given by the composition of a translation by $y \in \mathbb{R}^4$ with a homothety by $\lambda \in \mathbb{R}^+$. The pullback connection $t^*_{\lambda,y}A_0$ is still anti-self-dual; more explicitly,

$$A_{\lambda,y} = t^*_{\lambda,y}A_0 = \frac{\lambda^2}{\lambda^2 + |x-y|^2} \cdot \mathrm{Im}(q\,\mathrm{d}\bar{q})$$

$$F_{A_{\lambda,y}} = \left(\frac{\lambda^2}{\lambda^2 + |x-y|^2}\right)^2 \cdot \mathrm{Im}(\mathrm{d}q \wedge \mathrm{d}\bar{q})$$

Note that the action density function $|F_A|^2$ has again a bell-shaped profile centered at y and decays like r^{-4}; the parameter λ measures the concentration of the energy density function, and can be interpreted as the "size" of the instanton $A_{\lambda,y}$.

Instantons of topological charge k can be obtained by "superimposing" k basic instantons, via the so-called 't Hooft ansatz. Consider the function $\rho: \mathbb{R}^4 \to \mathbb{R}$ given by

$$\rho(x) = 1 + \sum_{j=1}^{k} \frac{\lambda_j^2}{(x-y_j)^2}$$

where $\lambda_j \in \mathbb{R}$ and $y_j \in \mathbb{R}^4$. Then the connection 1-form $A = A_\mu \mathrm{d}x_\mu$ with coefficients

$$A_\mu = i\sum_{\nu=1}^{4} \bar{\sigma}_{\mu\nu} \frac{\partial}{\partial x_\nu} \ln(\rho(x)) \qquad [8]$$

is anti-self dual; here, $\bar{\sigma}_{\mu\nu}$ are the matrices given by ($\mu, \nu = 1, 2, 3$):

$$\sigma_{\mu\nu} = \frac{1}{4\mathrm{i}}[\sigma_\mu, \sigma_\nu] \qquad \bar{\sigma}_{\mu 4} = \frac{1}{2}\sigma_\mu$$

where σ_μ are the Pauli matrices.

The connection [8] correspond to k instantons centered at points y_i with size λ_i. The basic instanton [6] is exactly (modulo gauge transformation) what one obtains from [8] for the case $k = 1$. The 't Hooft instantons form a $5k$-parameter family of anti-self-dual connections.

SU(2) instantons are also the building blocks for instantons with general structure group (Bernard *et al.* 1977). Let G be a compact semisimple Lie group, with Lie algebra $\mathfrak{g}$. Let $\phi: \mathfrak{su}(2) \to \mathfrak{g}$ be any injective Lie algebra homomorphism. If A is an anti-self-dual SU(2) connection 1-form, then it is easy to see that $\phi(A)$ is an anti-self-dual G-connection 1-form. Using [8] as an example, we have that

$$A = \mathrm{i}\sum_{\mu,\nu} \phi(\bar{\sigma}_{\mu\nu}) \frac{\partial}{\partial x_\nu} \ln(\rho(x))\mathrm{d}x_\mu \qquad [9]$$

is a G-instanton on $\mathbb{R}^4$.

While this guarantees the existence of G-instantons on $\mathbb{R}^4$, note that the instanton [9] might be reducible (e.g., ϕ can simply be the obvious inclusion of $\mathfrak{su}(2)$ into $\mathfrak{su}(n)$ for any n) and that its charge depends on the choice of representation ϕ. Furthermore, it is not clear whether every G-instanton can be obtained in this way, as the inclusion of a SU(2) instanton through some representation $\phi: \mathfrak{su}(2) \to \mathfrak{g}$.

The ADHM Construction

All SU(r) instantons on $\mathbb{R}^4$ can be obtained through a remarkable construction due to Atiyah, Drinfeld, Hitchin, and Manin. It starts by considering Hermitian vector spaces V and W of dimension c and r, respectively, and the following data (the so-called ADHM data):

$$B_1, B_2 \in \mathrm{End}(V), \ i \in \mathrm{Hom}(W, V)$$
$$j \in \mathrm{Hom}(V, W)$$

Assume, moreover, that (B_1, B_2, i, j) satisfy the ADHM equations:

$$[B_1, B_2] + ij = 0 \qquad [10]$$

$$[B_1, B_1^\dagger] + [B_2, B_2^\dagger] + ii^\dagger - j^\dagger j = 0 \qquad [11]$$

Now consider the following maps

$$\alpha: V \times \mathbb{R}^4 \to (V \oplus V \oplus W) \times \mathbb{R}^4$$
$$\beta: (V \oplus V \oplus W) \times \mathbb{R}^4 \to V \times \mathbb{R}^4$$

given as follows ($\mathbf{1}$ denotes the appropriate identity matrix):

$$\alpha(z_1, z_2) = \begin{pmatrix} B_1 + z_1\mathbf{1} \\ B_2 + z_2\mathbf{1} \\ j \end{pmatrix} \qquad [12]$$

$$\beta(z_1, z_2) = (-B_2 - z_2\mathbf{1} \quad B_1 + z_1\mathbf{1} \quad \mathrm{i}) \qquad [13]$$

where $z_1 = x_1 + \mathrm{i}x_2$ and $z_2 = x_3 + \mathrm{i}x_4$ are complex coordinates on $\mathbb{R}^4$. The maps [12] and [13] should be understood as a family of linear maps parametrized by points in $\mathbb{R}^4$.

A straightforward calculation shows that the ADHM equation [10] implies that $\beta\alpha = 0$ for every $(z_1, z_2) \in \mathbb{R}^4$. Therefore, the quotient $E = \ker\beta/\mathrm{im}\ \alpha = \ker\beta \cap \ker\alpha^\dagger$ forms a complex vector bundle over $\mathbb{R}^4$ or rank r whenever (B_1, B_2, i, j) is such that α is injective and β is surjective for every $(z_1, z_2) \in \mathbb{R}^4$.

To define a connection on E, note that E can be regarded as a sub-bundle of the trivial bundle $(V \oplus V \oplus W) \times \mathbb{R}^4$. So let $\iota : E \to (V \oplus V \oplus W) \times \mathbb{R}^4$ be the inclusion, and let $P : (V \oplus V \oplus W) \times \mathbb{R}^4 \to E$ be the orthogonal projection onto E. We can then define a connection ∇ on E through the projection formula

$$\nabla s = P\underline{d}\iota(s)$$

where $\underline{d}$ denotes the trivial connection on the trivial bundle $(V \oplus V \oplus W) \times \mathbb{R}^4$.

To see that this connection is anti-self-dual, note that projection P can be written as follows:

$$P = \mathbf{1} - \mathcal{D}^\dagger \Xi^{-1} \mathcal{D}$$

where

$$\mathcal{D} : (V \oplus V \oplus W) \times \mathbb{R}^4 \to (V \oplus V) \times \mathbb{R}^4$$

$$\mathcal{D} = \begin{pmatrix} \beta \\ \alpha^\dagger \end{pmatrix}$$

and $\Xi = \mathcal{D}\mathcal{D}^\dagger$. Note that $\mathcal{D}$ is surjective, so that Ξ is indeed invertible. Moreover, it also follows from [11] that $\beta\beta^\dagger = \alpha^\dagger\alpha$, so that $\Xi^{-1} = (\beta\beta^\dagger)^{-1}\mathbf{1}$.

The curvature F_∇ is given by

$$\begin{aligned} F_\nabla &= P\left(\underline{d}(\mathbf{1} - \mathcal{D}_1^\dagger \Xi^{-1}\mathcal{D})\underline{d}\right) = P(\underline{d}\mathcal{D}^\dagger \Xi^{-1}(\underline{d}\mathcal{D})) \\ &= P((\underline{d}\mathcal{D}^\dagger)\Xi^{-1}(\underline{d}\mathcal{D}) + \mathcal{D}^\dagger \underline{d}(\Xi^{-1}(\underline{d}\mathcal{D})) \\ &= (\underline{d}\mathcal{D}^\dagger)\Xi^{-1}(\underline{d}\mathcal{D}) \end{aligned}$$

for $P(\mathcal{D}^\dagger \underline{d}(\Xi^{-1}(\underline{d}\mathcal{D}))) = 0$ on $E = \ker\mathcal{D}$. Since Ξ^{-1} is diagonal, we conclude that F_∇ is proportional to $d\mathcal{D}^\dagger \wedge d\mathcal{D}$, as a 2-form.

It is then a straightforward calculation to show that each entry of $d\mathcal{D}^\dagger \wedge d\mathcal{D}$ belongs to $\Omega^{2,-}$.

The extraordinary accomplishment of Atiyah, Drinfeld, Hitchin, and Manin was to show that every instanton, up to gauge equivalence, can be obtained in this way (see, e.g., Donaldson and Kronheimer 1990). For instance, the basic SU(2) instanton [6] is associated with the following data ($c = 1, r = 2$):

$$B_1, B_2 = 0, \quad i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad j = (0 \quad 1)$$

Remark The ADHM data (B_1, B_2, i, j) are said to be stable if β is surjective for every $(z_1, z_2) \in \mathbb{R}^4$, and it is said to be costable if α is injective for every $(z_1, z_2) \in \mathbb{R}^4$. (B_1, B_2, i, j) is regular if it is both stable and costable. The quotient:

$$\{\text{regular solutions of (10) and (11)}\}/U(V)$$

coincides with the moduli space of instantons of rank $r = \dim W$ and charge $c = \dim V$ on $\mathbb{R}^4$ (see below). It is also an example of a quiver variety (*see* Finite Dimensional Algebras and Quivers), associated to the quiver consisting of two vertices V and W, two loop-edges on the vertex V and two edges linking V to W, one in each direction.

Dimensional Reductions of the Anti-Self-Dual Yang–Mills Equation

As pointed out above, a connection on a Hermitian vector bundle $E \to \mathbb{R}^4$ of rank r can be regarded as 1-form

$$A = \sum_{k=1}^{4} A_k(x_1, \ldots, x_4)\mathrm{d}x^k, \quad A_k : \mathbb{R}^4 \to \mathfrak{u}(r)$$

Assuming that the connection components A_k are invariant under translation in one direction, say x_4, we can think of

$$\underline{A} = \sum_{k=1}^{3} A_k(x_1, x_2, x_3)\mathrm{d}x^k$$

as a connection on a Hermitian vector bundle over $\mathbb{R}^3$, with the fourth component $\phi = A_4$ being regarded as a bundle endomorphism $\phi : E \to E$, called a Higgs field. In this way, the anti-self-duality equation [3] reduces to the so-called Bogomolny (or monopole) equation:

$$F_{\underline{A}} = *\mathrm{d}\phi \qquad [14]$$

where $*$ is the Euclidean Hodge star in dimension 3.

Now assume that the connection components A_k are invariant under translation in two directions, say x_3 and x_4. Consider

$$\underline{A} = \sum_{k=1}^{2} A_k(x_1, x_2)\mathrm{d}x^k$$

as a connection on a Hermitian vector bundle over $\mathbb{R}^2$, with the third and fourth components combined into a complex bundle endomorphism:

$$\Phi = (A_3 + \mathrm{i} \cdot A_4)(\mathrm{d}x_1 - \mathrm{i} \cdot \mathrm{d}x_2)$$

taking values on 1-forms. The anti-self-duality equation [3] is then reduced to the so-called Hitchin's equations:

$$F_{\underline{A}} = [\Phi, \Phi^*], \qquad \bar{\partial}_{\underline{A}}\Phi = 0 \qquad [15]$$

Conformal invariance of the anti-self-duality equation means that Hitchin's equations are well defined over any Riemann surface.

Finally, assume that the connection components A_k are invariant under translation in three directions, say x_2, x_3, and x_4. After gauging away the first component A_1, the anti-self-duality equations [3] reduce to the so-called Nahm's equations:

$$\frac{\mathrm{d}T_k}{\mathrm{d}x_1} + \frac{1}{2}\sum_{j,l} \epsilon_{kjl}[T_j, T_l] = 0, \quad j,k,l = \{2,3,4\} \qquad [16]$$

where each T_k is regarded as a map $\mathbb{R} \to \mathfrak{u}(r)$.

Readers who are interested in monopoles and Nahm's equations are referred to the survey by Murray (2002) and references therein. The best source for Hitchin's equations still are Hitchin's (1987a, b) original papers. A beautiful duality, known as Nahm transform, relates the various reductions of the anti-self-duality equation to periodic instantons; see the survey article by Jardim (2004).

It is also worth mentioning the book by Mason and Woodhouse (1996), where other interesting dimensional reductions of the anti-self-duality equation are discussed, providing a deep relation between instantons and the general theory of integrable systems.

The Instanton Moduli Space

Now fix a rank-r complex vector bundle E over a four-dimensional Riemannian manifold X. Observe that the difference between any two connections is a linear operator:

$$(\nabla - \nabla')(f\sigma) = f\nabla\sigma + \sigma \cdot \mathrm{d}f - f\nabla'\sigma - \sigma \cdot \mathrm{d}f$$
$$= f(\nabla - \nabla')\sigma$$

In other words, any two connections on E differ by an endomorphism-valued 1-form. Therefore, the set of all smooth connections on E, denoted by $\mathcal{A}(E)$, has the structure of an affine space over $\Gamma(\mathrm{End}(E)) \otimes \Omega^1_M$.

The gauge group $\mathcal{G}(E)$ acts on $\mathcal{A}(E)$ via conjugation:

$$g \cdot \nabla := g^{-1}\nabla g$$

We can form the quotient set $\mathcal{B}(E) = \mathcal{A}(E)/\mathcal{G}(E)$, which is the set of gauge equivalence classes of connections on E.

The set of gauge equivalence classes of anti-self-dual connections on E is a subset of $\mathcal{B}(E)$, and it is called the moduli space of instantons on $E \to X$. The subset of $\mathcal{M}_X(E)$ consisting of irreducible anti-self-dual connections is denoted $\mathcal{M}^*_X(E)$.

Since the choice of a particular vector bundle within its topological class is immaterial, these sets are usually labeled by the topological invariants (Chern or Pontrjagyn classes) of the bundle E. For instance, $\mathcal{M}(r,k)$ denotes the moduli space of instantons on a rank-r complex vector bundle $E \to X$ with $c_1(E) = 0$ and $c_2(E) = k > 0$. It turns out that $\mathcal{M}_X(E)$ can be given the structure of a Hausdorff topological space. In general, $\mathcal{M}_X(E)$ will be singular as a differentiable manifold, but $\mathcal{M}^*_X(E)$ can always be given the structure of a smooth Riemannian manifold.

We start by explaining the notion of a L^2_p vector bundle. Recall that $L^2_p(\mathbb{R}^n)$ denotes the completion of the space of smooth functions $f : \mathbb{R}^n \to \mathbb{C}$ with respect to the norm:

$$\|f\|^2_{L^2_p} = \int_X (|f|^2 + |\mathrm{d}f|^2 + \cdots + |\mathrm{d}^{(p)}f|^2)$$

In dimension $n = 4$ and for $p > 2$, by virtue of the Sobolev embedding theorem, L^2_p consists of continuous functions, i.e., $L^2_p(\mathbb{R}^n) \subset C^0(\mathbb{R}^n)$. So we define the notion of a L^2_p vector bundle as a topological vector bundle whose transition functions are in L^2_p, where $p > 2$.

Now for a fixed L^2_p vector bundle E over X, we can consider the metric space $\mathcal{A}_p(E)$ of all connections on E which can be represented locally on an open subset $U \subset X$ as a $L^2_p(U)$ 1-form. In this topology, the subset of irreducible connections $\mathcal{A}^*_p(E)$ becomes an open dense subset of $\mathcal{A}_p(E)$. Since any topological vector bundle admits a compatible smooth structure, we may regard L^2_p connections as those that differ from a smooth connection by a L^2_p 1-form. In other words, $\mathcal{A}_p(E)$ becomes an affine space modeled over the Hilbert space of L^2_p 1-forms with values in the endomorphisms of E. The curvature of a connection in $\mathcal{A}_p(E)$ then becomes a L^2_{p-1} 2-form with values in the endomorphism bundle $\mathrm{End}(E)$.

Moreover, let $\mathcal{G}_{p+1}(E)$ be defined as the topological group of all L^2_{p+1} bundle automorphisms. By virtue of the Sobolev multiplication theorem, $\mathcal{G}_{p+1}(E)$ has the structure of an infinite-dimensional

Lie group modeled on a Hilbert space; its Lie algebra is the space of L^2_{p+1} sections of End(E).

The Sobolev multiplication theorem is once again invoked to guarantee that the action $\mathcal{G}_{p+1}(E) \times \mathcal{A}_p(E) \to \mathcal{A}_p(E)$ is a smooth map of Hilbert manifolds. The quotient space $\mathcal{B}_p(E) = \mathcal{A}_p(E)/\mathcal{G}_{p+1}(E)$ inherits a topological structure; it is a metric (hence Hausdorff) topological space. Therefore, the subspace $\mathcal{M}_X(E)$ of $\mathcal{B}_p(E)$ is also a Hausdorff topological space; moreover, one can show that the topology of $\mathcal{M}_X(E)$ does not depend on p.

The quotient space $\mathcal{B}_p(E)$ fails to be a Hilbert manifold because in general the action of $\mathcal{G}_{p+1}(E)$ on $\mathcal{A}_p(E)$ is not free. Indeed, if A is a connection on a rank-r complex vector bundle E over a connected base manifold X, which is associated with a principal G-bundle. Then the isotropy group of A within the gauge group

$$\Gamma_A = \{g \in \mathcal{G}_{p+1}(E) | g(A) = A\}$$

is isomorphic to the centralizer of the holonomy group of A within G.

This means that the subspace of irreducible connections $\mathcal{A}^*_p(E)$ can be equivalently defined as the open dense subset of $\mathcal{A}_p(E)$ consisting of those connections whose isotropy group is minimal, that is,

$$\mathcal{A}^*_p(E) = \{A \in \mathcal{A}_p(E) | \Gamma_A = \text{center}(G)\}$$

Now $\mathcal{G}_{p+1}(E)$ acts with constant isotropy on $\mathcal{A}^*_p(E)$; hence, the quotient $\mathcal{B}^*_p(E) = \mathcal{A}^*_p(E)/\mathcal{G}_{p+1}(E)$ acquires the structure of a smooth Hilbert manifold.

Remark The analysis of neighborhoods of points in $\mathcal{B}_p(E) \backslash \mathcal{B}^*_p(E)$ is very relevant for applications of the instanton moduli spaces to differential topology. The simplest situation occurs when A is an SU(2) connection on a rank-2 complex vector bundle E which reduces to a pair of U(1) and such $[A]$ occurs as an isolated point in $\mathcal{B}_p(E) \backslash \mathcal{B}^*_p(E)$. Then a neighborhood of $[A]$ in $\mathcal{B}_p(E)$ looks like a cone on an infinite-dimensional complex projective space.

Alternatively, the instanton moduli space $\mathcal{M}_X(E)$ can also be described by first taking the subset of all anti-self-dual connections and then taking the quotient under the action of the gauge group. More precisely, consider the map

$$\begin{aligned} \rho : \mathcal{A}_p(E) &\to L^2_p(\text{End}(E) \otimes \Omega^{2,+}_X) \\ \rho(A) &= F^+_A \end{aligned} \qquad [17]$$

Thus, $\rho^{-1}(0)$ is exactly the set of all anti-self-dual connections. It is $\mathcal{G}_{p+1}(E)$-invariant, so we can take the quotient to get

$$\mathcal{M}_X(E) = \rho^{-1}(0)/\mathcal{G}_{p+1}(E)$$

It follows that the subspace $\mathcal{M}^*_X(E) = \mathcal{B}^*_p(E) \cap \mathcal{M}_X(E)$ has the structure of a smooth Hilbert manifold. Index theory comes into play to show that $\mathcal{M}^*_X(E)$ is finite dimensional. Recall that if D is an elliptic operator on a vector bundle over a compact manifold, then D is Fredholm (i.e., ker D and coker D are finite dimensional) and its index

$$\text{ind}\, D = \dim \ker D - \dim \text{coker}\, D$$

can be computed in terms of topological invariants, as prescribed by the Atiyah–Singer index theorem. The goal here is to identify the tangent space of $\mathcal{M}^*_X(E)$ with the kernel of an elliptic operator.

It is clear that, for each $A \in \mathcal{A}_p(E)$, the tangent space $T_A\mathcal{A}_p(E)$ is just $L^2_p(\text{End}(E) \otimes \Omega^1_X)$. We define the pairing

$$\langle a, b \rangle = \int_X a \wedge *b \qquad [18]$$

and it is easy to see that this pairing defines a Riemannian metric (the so-called L^2-metric) on $\mathcal{A}_p(E)$.

The derivative of the map ρ in [17] at the point A is given by

$$\begin{aligned} d^+_A : L^2_p(\text{End}(E) \otimes \Omega^1_X) &\to L^2_{p-1}(\text{End}(E) \otimes \Omega^2_X) \\ a &\mapsto (d_A a)^+ \end{aligned}$$

so that for each $A \in \rho^{-1}(0)$ we have

$$T_A\rho^{-1}(0) = \left\{a \in L^2_p(\text{End}(E)) \otimes \Omega^1_X \,|\, d^+_A a = 0\right\}$$

Now for a gauge equivalence class $[A] \in \mathcal{B}^*_p(E)$, the tangent space $T_{[A]}\mathcal{B}^*_p(E)$ consists of those 1-forms which are orthogonal to the fibers of the principal $\mathcal{G}_{p+1}(E)$ bundle $\mathcal{A}^*_p(E) \to \mathcal{B}^*_p(E)$. At a point $A \in \mathcal{A}_p(E)$, the derivative of the action by some $g \in \mathcal{G}_{p+1}(E)$ is

$$-d_A \;:\; L^2_{p+1}(\text{End}(E)) \to L^2_p(\text{End}(E) \otimes \Omega^1_X)$$

Usual Hodge decomposition gives us that there is an orthogonal decomposition:

$$L^2_p(\text{End}(E) \otimes \Omega^1_X) = \text{im}\, d_A \oplus \ker d^*_A$$

which means that:

$$T_{[A]}\mathcal{B}^*_p(E) = \left\{a \in L^2_p(\text{End}(E) \otimes \Omega^1_X) \,|\, d^*_A a = 0\right\}$$

Thus, the pairing [18] also defines a Riemannian metric on $\mathcal{B}^*_p(E)$. Putting these together, we conclude that the space $T_{[A]}\mathcal{M}^*_X$ tangent to $\mathcal{M}^*_X(E)$ at an equivalence class $[A]$ of anti-self-dual connections can be described as follows:

$$\begin{aligned} &T_{[A]}\mathcal{M}^*_X(E) \\ &= \left\{a \in L^2_p(\text{End}(E) \otimes \Omega^1_X) \,|\, d^*_A a = d^+_A a = 0\right\} \end{aligned} \qquad [19]$$

It turns out that the so-called deformation operator $\delta_A = d_A^* \oplus d_A$:

$$\delta_A : L_p^2(\mathrm{End}(E) \otimes \Omega_X^1) \rightarrow L_{p+1}^2(\mathrm{End}(E)) \oplus L_{p-1}^2(\mathrm{End}(E) \otimes \Omega_X^2)$$

is elliptic. Moreover, if A is anti-self-dual then coker δ_A is empty, so that $T_{[A]}\mathcal{M}_X^*(E) = \ker \delta_A$. The dimension of the tangent space $T_{[A]}\mathcal{M}_X^*(E)$ is then simply given by the index of the deformation operator δ_A. Using the Atiyah–Singer index theorem, we have for SU(r) bundles with $c_2(E) = k$:

$$\dim \mathcal{M}_X^*(E) = 4rk - (r^2 - 1)(1 - b_1(X) + b_+(X))$$

The dimension formula for arbitrary gauge group G can be found in Atiyah *et al.* (1978).

For example, the moduli space of SU(2) instantons on $\mathbb{R}^4$ of charge k is a smooth Riemannian manifold of dimension $8k - 3$. These parameters are interpreted as the $5k$ parameters describing the positions and sizes of k separate instantons, plus $3(k - 1)$ parameters describing their relative SU(2) phases.

The detailed construction of the instanton moduli spaces can be found in Donaldson and Kronheimer (1990). An alternative source is Morgan's lecture notes (Friedman and Morgan 1998). It is interesting to note that $\mathcal{M}_X^*(E)$ inherits many of the geometrical properties of the original manifold X. Most notably, if X is a Kähler manifold, then $\mathcal{M}_X^*(E)$ is also Kähler; if X is a hyper-Kähler manifold, then $\mathcal{M}_X^*(E)$ is also hyper-Kähler. One expects that other geometric structures on X can also be transferred to the instanton moduli spaces $\mathcal{M}_X^*(E)$.

See also: Characteristic Classes; Finite-Dimensional Algebras and Quivers; Gauge Theoretic Invariants of 4-Manifolds; Gauge Theory: Mathematical Applications; Integrable Systems: Overview; Index Theorems; Moduli Spaces: An Introduction; Solitons and Other Extended Field Configurations; Twistor Theory: Some Applications [in Integrable Systems, Complex Geometry and String Theory].

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Integrability and Quantum Field Theory

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Introduction

The notion of integrability plays many different rôles in quantum field theory (QFT). In this article we interpret it in a narrow sense and describe some QFTs that are completely integrable, in the sense that there are as many integrals of motion as degrees of freedom. Necessarily this implies, since we are talking about field theories, that there is an infinite number of conserved quantities. The existence of such a tower of conserved quantities of increasing Lorentz spin implies, via the Coleman–Mandula theorem, that the theories are trivial in spacetime dimensions greater than 2. On the other hand, in $1 + 1$ dimensions there is a rich menagerie of such integrable quantum field theories (IQFTs). These theories are fascinating in their own right as nontrivial QFTs for which data like the S-matrix and spectrum can be determined exactly. We will describe these exact S-matrices for a series of seminal examples. In addition, we briefly describe the applications of these theories to statistical systems in two dimensions.

Classical Integrable Systems and Field Theories

For a field theory to be integrable it must have an infinite number of conserved charges. Necessarily these must be spacetime symmetries which extend the Poincaré symmetry in some way. It turns out that, due to a theorem of Coleman and Mandula, such

extensions are very restrictive: they are only possible in $1+1$ dimensions (one dimension of space and one of time) apart from noninteracting theories. Below we describe some of the most important examples.

Affine Toda Theories

These theories describe the interactions of a set of scalar fields which we write as a vector $\boldsymbol{\phi}$. The action is

$$S = \int d^2x \left(\frac{1}{2}(\partial_\mu \boldsymbol{\phi})^2 - V(\boldsymbol{\phi})\right) \qquad [1]$$

The potential has to be very specially chosen in order that the resulting theory is integrable. The resulting theories are classified by affine Lie algebras. We shall describe only the theories related to a simply laced Lie algebra $\mathfrak{g}$ (so of ADE type). In this case, for the affine version of the theory,

$$V(\boldsymbol{\phi}) = \frac{m^2}{\beta^2}\sum_{a=0}^{r} n_a\, e^{\beta\boldsymbol{\alpha}_a\cdot\boldsymbol{\phi}} \qquad [2]$$

where $\boldsymbol{\phi}$ is an r-rank $\mathfrak{g}$ vector and $\boldsymbol{\alpha}_a, a=1,\ldots,r$, are a set of simple roots of $\mathfrak{g}$. The fact that we are considering the affine version of the theory means that we include the term involving the extended root (the lowest root) $\boldsymbol{\alpha}_0 = -\sum_{a=1}^{r} n_a\boldsymbol{\alpha}_a$, which defines the integers $n_a (n_0 = 1)$. If this term is absent then the potential does not have a minimum. Such nonaffine theories are interesting in their own right since they include the Liouville theory, but we shall not describe them here.

One way to expose the infinite set of conserved charges at the classical level is to write the equations of motion in Lax form. This has the form of the vanishing of the field strength, or zero-curvature condition, of an auxiliary gauge connection in $\mathfrak{g}$ with components (A_x, A_t):

$$\begin{aligned} A_x &= \partial_t\boldsymbol{\phi}\cdot\boldsymbol{H} + \frac{m}{2\beta}\sum_{a=0}^{r} e^{\beta\boldsymbol{\alpha}_a\cdot\boldsymbol{\phi}/2}(e_a + f_a) \\ A_t &= \partial_x\boldsymbol{\phi}\cdot\boldsymbol{H} + \frac{m}{2\beta}\sum_{a=0}^{r} e^{\beta\boldsymbol{\alpha}_a\cdot\boldsymbol{\phi}/2}(e_a - f_a) \end{aligned} \qquad [3]$$

Here, $\{e_i, f_i\}$ are related to generators of $\mathfrak{g}$ in a Cartan–Weyl basis, via

$$\begin{aligned} e_a &= zE_{\boldsymbol{\alpha}_a}, \quad f_a = z^{-1}E_{-\boldsymbol{\alpha}_a}, \qquad a = 1,\ldots,r \\ e_0 &= z^{-h}E_{\boldsymbol{\alpha}_0}, \quad f_0 = z^{h}E_{-\boldsymbol{\alpha}_0} \end{aligned} \qquad [4]$$

where z is a auxiliary variable known as the spectral parameter and h is the Coxeter number of $\mathfrak{g}$. Using the following commutators of $\mathfrak{g}$,

$$\begin{aligned} [E_{\boldsymbol{\alpha}_a}, E_{\boldsymbol{\alpha}_b}] &= \delta_{ab}\boldsymbol{\alpha}_a\cdot\boldsymbol{H} \\ [\boldsymbol{H}, E_{\boldsymbol{\alpha}}] &= \boldsymbol{\alpha}E_{\boldsymbol{\alpha}} \\ [E_{\boldsymbol{\alpha}_a}, E_{-\boldsymbol{\alpha}_b}] &= 0 \end{aligned} \qquad [5]$$

it is straightforward to verify that the zero-curvature condition

$$F_{xt} = \partial_x A_t - \partial_t A_x + [A_x, A_t] = 0 \qquad [6]$$

is equivalent to the equations of motion which follow from extremizing the action [1].

The fact that there exists a flat connection which depends on an auxiliary parameter z is sufficient to ensure integrability. In brief, the idea is that the gauge connection can be "abelianized" by a gauge transformation:

$$\tilde{A}_\mu = U\partial_\mu U^{-1} + UA_\mu U^{-1} \quad \text{with } [\tilde{A}_t, \tilde{A}_x] = 0 \qquad [7]$$

Hence, $\partial_t\tilde{A}_x - \partial_x\tilde{A}_t = 0$. This can be done in two inequivalent ways, such that $\tilde{A}_\mu$ are polynomials in z and z^{-1}, respectively. The corresponding coefficients are then conserved currents whose integrals give conserved charges. It can be shown that for the Toda theories these conserved charges have Lorentz spin given by an exponent $\{s_a\}$ of $\mathfrak{g}$ modulo its Coxeter number h:

$$\begin{array}{lll} A_n: & h=n+1, & \{1,2,3,\ldots,n\} \\ D_n: & h=2n-2, & \{1,3,5,\ldots,2n-3,n-1\} \\ E_6: & h=12, & \{1,4,5,7,8,11\} \\ E_7: & h=18, & \{1,5,7,9,11,13,17\} \\ E_8: & h=30, & \{1,7,11,13,17,19,23,29\} \end{array} \qquad [8]$$

This spectrum of conserved quantities seems to be a ubiquitous feature of IQFTs. These theories can be generalized by replacing $\mathfrak{g}$, or rather its (untwisted affinization) with any affine algebra.

The Sinh/Sine-Gordon Theory

These theories are the simplest of the Toda theories described above, associated to the Lie algebra A_1. In this case there is a single field and the potential has the form

$$V(\phi) = \frac{m^2}{2\beta^2}\left(e^{\beta\phi} + e^{-\beta\phi}\right) \qquad [9]$$

We have rescaled the field by $1/\sqrt{2}$ relative to the normalization in [2]. This potential defines the "sinh-Gordon theory." However, we can also take $\beta \to i\beta$ to give the sine-Gordon theory with an action

$$S = \int d^2x \left(\frac{1}{2}(\partial_\mu\phi)^2 + \frac{m^2}{\beta^2}\cos(\beta\phi)\right) \qquad [10]$$

The sine-Gordon theory is a useful paradigm for IQFTs because it exhibits most of the features of more complicated examples. To start with, it illustrates another important property of some integrable systems; namely, the existence of solitons. In the sine-Gordon case, the minima of the potential lie at $\phi = 2n\pi/\beta$, for an integer n, so there is a topological

kink that separates a vacuum n on the left and $n+1$ on the right, as well as an antikink. The explicit solution for the kink moving with velocity v is

$$\phi(x,t) = \frac{4}{\beta}\tan^{-1}\exp(m(x\cosh\theta - t\sinh\theta - \xi)) \quad [11]$$

where ξ is a constant and, since we are working in $1+1$ dimensions, we have introduced the rapidity θ, in terms of which the velocity is

$$v = \tanh\theta, \qquad -\infty \leq \theta \leq \infty \quad [12]$$

The antikink solution is simply the negative of the above. The kinks have a mass

$$M = \frac{8m}{\beta^2} \quad [13]$$

The existence of topological solitons is not a consequence of integrability, *per se*, for example, the ϕ^4 theory in $1+1$ dimensions also has kinks; however, in the integrable setting, the solitons have special properties that survive in the quantum theory. The first property is that multisoliton solutions can be found exactly using a variety of different techniques. They are most easily written down using the tau function, which is related to the field via

$$\phi = -\frac{1}{i\beta}\log\frac{\tau}{\tau^*} \quad [14]$$

The N-soliton solution can then be written compactly as

$$\tau = \sum_{\{\mu_p\}=0,1} \exp\left(\sum_{p=1}^{N} \mu_p \Phi^{(p)} + \sum_{p,q=1}^{N} \mu_p\mu_q \Upsilon^{(pq)}\right) \quad [15]$$

The sum is over the 2^N possibilities for which $\mu_p = 0$ or 1, for each p, and we have introduced

$$\Phi^{(p)} = m(x\cosh\theta_p - t\sinh\theta_p - \xi_p) \pm \frac{i\pi}{2} \quad [16]$$

The rapidity of the pth soliton is θ_p, and the choice of sign corresponds to the kink and antikink, respectively. The "interaction coefficient" is

$$\exp\Upsilon^{(pq)} = \tanh^2\left(\tfrac{1}{2}(\theta_p - \theta_q)\right) \quad [17]$$

For example, the two-soliton solution is

$$\tau = 1 + e^{\Phi^{(1)}} + e^{\Phi^{(2)}} + e^{\Upsilon + \Phi^{(1)} + \Phi^{(2)}} \quad [18]$$

The multisoliton solutions have a natural physical interpretation as the histories of a set of solitons which scatter off each other. To make this more precise, consider the two-soliton solution [18] in more detail. Suppose that $\xi_1 < \xi_2, v_1 > v_2$. Focus on the solution in the vicinity of the first soliton, that is,

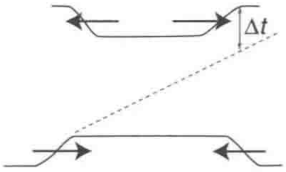


Figure 1 Classical scattering of a kink and an antikink. The final velocities equal the initial velocities and the only effect is to introduce a velocity-dependent time delay as shown.

$x \sim v_1 t + \xi_1$. In the limit $t \to -\infty$, the solution is approximately

$$\tau \simeq 1 + e^{\Phi^{(1)}} \quad [19]$$

while, as $t \to \infty$, it is approximately

$$\tau \simeq e^{\Phi^{(2)}}\left(1 + e^{\Upsilon + \Phi^{(1)}}\right) \quad [20]$$

In both the limits, the solution represents an isolated soliton, the only difference is that the final "position offset" has been displaced: $\xi_1 \longmapsto \xi_1 - \Upsilon$. It is a consequence of integrability that the solitons interact in such a simple way. There were two solitons in the initial configuration and two in the final configuration traveling with the same velocities. The only effect is to introduce a time delay of

$$\Delta t = -\frac{\Upsilon(\theta)}{m\sinh(\theta/2)} \quad [21]$$

in the center-of-mass frame with $\theta_1 = -\theta_2 = \theta/2$, which we illustrate in **Figure 1**. We shall see that this kind of simple scattering is a characteristic feature of integrable field theories which extends to the quantum theory. It reflects the enormous restriction that the existence of the infinite set of integrals of motion puts on the dynamics.

Integrability at the Quantum Level

In this section we turn to the particular implications of integrability for the field theories at the quantum level. In discussing theories in $1+1$ dimensions it is convenient, as in [12], to use the rapidity. The energy and momentum of a particle of mass m are $E = m\cosh\theta$ and $p = m\sinh\theta$, respectively.

The sinh- and sine-Gordon theory, and their affine Toda generalizations, are scalar field theories with a well-behaved potential and as such they can be quantized in the conventional manner. It can be shown that integrability survives quantization and we now address its consequences. The key observation is that having an infinite set of higher-spin conserved quantities is very restrictive on the possible quantum processes. Assuming that the theory has a mass gap, the asymptotic states $|a,\theta\rangle$ are particles with rapidity

θ and additional quantum numbers needed to specify the state are indicated by the label a. These states are eigenstates of the conserved charges,

$$Q_s|a,\theta\rangle = q_s(a)e^{s\theta}|a,\theta\rangle \qquad [22]$$

Here, s is the spin of the charge which ranges over some infinite subset of the integers. Since the charges must commute with the S-matrix, it follows immediately that if an incoming state of n particles has a set of rapidities $\{\theta_1,\ldots,\theta_n\}$ then the outgoing state must also have n particles with the same set $\{\theta_1,\ldots,\theta_n\}$: there is consequently no particle creation! For example, we have illustrated the scattering of two particles in **Figure 2**. The two-particle S-matrix element will be denoted as

$$S_{ab}^{cd}(\theta_1-\theta_2):\ |a,\theta_1;b,\theta_2\rangle \longrightarrow |c,\theta_2;d,\theta_1\rangle \qquad [23]$$

Note that masses of the incoming particles must match the outgoing ones: $m_a=m_d$ and $m_b=m_c$. We have already seen this kind of behavior with the classical scattering of solitons in the sine-Gordon theory. In spite of the fact that the scattering is purely elastic, it can be nontrivial for two reasons: if there are mass degeneracies in the theory, the quantum numbers $\{a_1,\ldots,a_n\}$ can change and, in addition, the S-matrix element can depend nontrivially on the momenta.

The fact that the incoming and outgoing states have the same set of momenta leads to the notion of factorizability. To see what this means, consider the case of three particles. Let us imagine that we prepare the initial state to consist of three fairly narrow wave packets in position space with momenta smeared in accordance with the uncertainty principle. The key to the following argument is the fact that the infinite set of higher-spin conserved charges (with commute with the S-matrix) allow one to move the positions of the three particles relative to each other in an arbitrary way. In addition, the theory has a mass gap, so interactions have a finite range. By using this freedom, we can arrange for particles 1 and 2 to interact first,

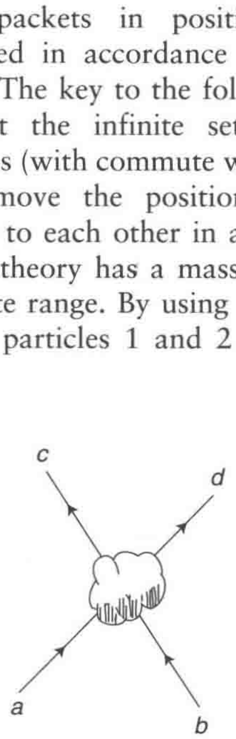


Figure 2 The two particle S-matrix with particles a and b in the initial state and c and d in the final state. For consistency, $m_a=m_d$ and $m_b=m_c$.

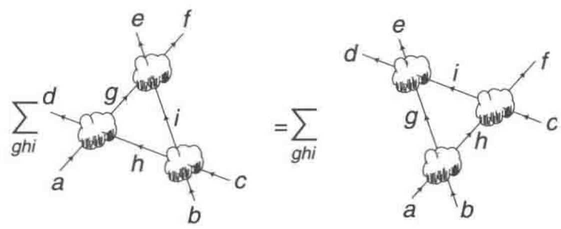


Figure 3 The scattering of three particles can factorize in two distinct ways as illustrated, leading to a nontrivial condition: the Yang–Baxter equation.

well before they come within interaction range of the third. Subsequently, the first two particles interact with the third as on the right-hand side of **Figure 3**. This ability to move the wave packets around using the symmetries means that the three-particle S-matrix element must "factorize" into a product of three two-particle elements:

$$S_{abc}^{def}(\theta_1,\theta_2,\theta_3) = \sum_{ghi} S_{ab}^{gh}(\theta_1-\theta_2)S_{hc}^{if}(\theta_1-\theta_3)S_{gi}^{de}(\theta_2-\theta_3) \qquad [24]$$

However, we could also use the symmetries afforded by the conserved charges to shift the positions of the particles so that particle 2 and 3 interact first, as on the left-hand side of **Figure 3**. Since the charges commute with the S-matrix, the result must the same; hence, there is a nontrivial consistency condition:

$$\sum_{ghi} S_{bc}^{hi}(\theta_2-\theta_2)S_{ah}^{dg}(\theta_1-\theta_3)S_{gi}^{ef}(\theta_2-\theta_3) = \sum_{ghi} S_{ab}^{gh}(\theta_1-\theta_2)S_{hc}^{if}(\theta_1-\theta_3)S_{gi}^{de}(\theta_2-\theta_3) \qquad [25]$$

This is the celebrated Yang–Baxter equation. Notice that it is only nontrivial if there are mass degeneracies, otherwise the particles on internal lines are determined by the external particles.

The factorization of the S-matrix extends readily to the case of more particles in an obvious way. An n-body element factorizes into a two-body element for each pair of particles. One might think that considerations of the n-particle S-matrix would lead to additional constraints; however, it can readily be shown that this is not the case and that the Yang–Baxter equation acts as a basic "move" which allows one to reorder the n-particle S-matrix into an arbitrary order. Further conditions on the S-matrix come from the axioms of analytic S-matrix theory:

(i) *Unitarity*

$$\sum_{ef} S_{ab}^{ef}(\theta)S_{ef}^{cd}(-\theta) = \delta_{ac}\delta_{bd} \qquad [26]$$

(ii) *Crossing symmetry* Each particle a has an antiparticle $\bar{a}$ and

$$S_{ab}^{cd}(\theta) = S_{b\bar{d}}^{\bar{a}c}(\pi i - \theta) \qquad [27]$$

(iii) *Analyticity* The S-matrix is a meromorphic function of θ on the physical strip, $0 \leq \operatorname{Im}\theta \leq \pi$. Singularities in most instances occur along the imaginary axis and the simple poles correspond to direct or cross-channel resonances. In this case, if $S_{ab}^{de}(\theta)$ has a simple pole at $\theta = \mathrm{i}u_{ab}^{c}$ (necessarily a nonphysical rapidity difference) in the direct channel there exists a bound state of a and b of mass

$$m_c^2 = m_a^2 + m_b^2 + 2m_a m_b \cos u_{ab}^c \qquad [28]$$

The situation is illustrated in **Figure 4**. The new particle must itself be included in the particle spectrum. The S-matrix elements at the pole have the form

$$S_{ab}^{de}(\theta) = \sum_c P_{ab}^c \frac{\mathrm{i}r_{ab}^c}{\theta - \mathrm{i}u_{ab}^c} P_{d\bar{e}}^{\bar{c}} + \cdots \qquad [29]$$

where P_{ab}^c can be thought of as a kind of projection operator with

$$\sum_{ab} P_{ab}^c P_{\bar{b}\bar{a}}^{\bar{d}} = \delta^{cd} \qquad [30]$$

Unitarity of the QFT requires that r_{ab}^c is real and positive, although there are also examples of nonunitarity theories with exact S-matrices. If $ab \to c$ can occur then so can $a\bar{c} \to \bar{b}$ and $b\bar{c} \to \bar{a}$. From [28], we deduce the following identity:

$$u_{ab}^c + u_{a\bar{c}}^{\bar{b}} + u_{b\bar{c}}^{\bar{a}} = 2\pi \qquad [31]$$

The data $\{u_{ab}^c\}$ for any given scattering theory are known as the fusing angles.

(iv) *The Bootstrap equations* These give a nonlinear relation between S-matrix elements. The basic idea is that if particle c appears as a resonance in the scattering of a and b then the S-matrix element of c with another state d can be deduced in terms of the scattering of d with a and b. This is illustrated in **Figure 5**. Using [30], we can write the resulting equation for the S-matrix element of c and d directly:

$$S_{cd}^{ef}(\theta) = \sum_{ghi} P_{\bar{a}\bar{b}}^{\bar{c}} S_{ab}^{eg}\left(\theta - \mathrm{i}\bar{u}_{a\bar{c}}^{\bar{b}}\right) S_{bd}^{hi}\left(\theta + \mathrm{i}\bar{u}_{b\bar{c}}^{\bar{a}}\right) P_{gi}^{f} \qquad [32]$$

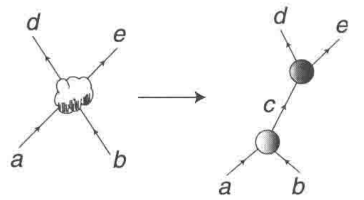


Figure 4 Near a direct channel pole, the scattering of *a* and *b* is dominated by the bound state *c*.

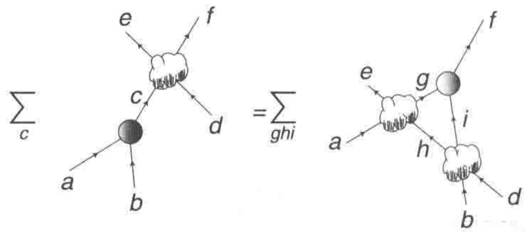


Figure 5 The bootstrap equations result from considering the interaction of a particle *d* with the bound state *c* of *a* and *b* in two distinct ways as illustrated.

The bootstrap constraints are very powerful because they allow one to extract the S-matrix elements of new particles that appear as bound states. This leads to the philosophy of the "bootstrap program" where one attempts to build consistent S-matrices starting from the S-matrix for a subset of particles which act as a seed for the algorithm. The process is quite an art, but at the end one has to be satisfied that the complete analytic structure is consistent with all the axioms. The key is to be able to account for all the poles in a consistent way, either in terms of bound states, as above, or in terms of the Coleman–Thun mechanism. This allows some poles to be interpreted in ways other than the existence of a bound state. The bootstrap algorithm is very complicated in general and at the present time a complete classification of solutions is not known. However, there are a large number of known solutions which appear to be intimately related to Lie algebras and associated structures known as Yangians and quantum groups. Below we describe some of the simplest known solutions.

Minimal *S*-Matrices

These scattering theories are in some sense the simplest. The particle spectrum is generally nondegenerate and so the Yang–Baxter equation is trivial. As is ubiquitous in the subject of IQFT, the classification of the theories is related to Lie algebras, although what seems to be important is not so much the algebra in question but rather the details of the associated root system. In this case the appropriate algebras are the simply laced algebras of ADE type. The number of particles is equal to the rank r of the Lie algebra and the masses are given by the r elements of one of the eigenvectors of the Cartan matrix of the algebra $\mathfrak{g}$:

$$\sum_{b=1}^{r} C_{ab} m_b = \left(2 - 2\cos\frac{\pi}{h}\right) m_a \qquad [33]$$

where h is the Coxeter number of $\mathfrak{g}$. The conserved charges have spins corresponding to the exponents of $\mathfrak{g}$ modulo h. We briefly explain how the complete

S-matrix can be written down in terms of properties of the root system of $\mathfrak{g}$. Let $\boldsymbol{\Phi}$ be the set of roots of $\mathfrak{g}$, and $\boldsymbol{\alpha}_a, a=1,\ldots,r$, a set of simple roots, as in the last section. In terms of these, $C_{ab}=2\boldsymbol{\alpha}_a\cdot\boldsymbol{\alpha}_b/\boldsymbol{\alpha}_b^2$. Let $\boldsymbol{\omega}_a, a=1,\ldots,r$, be a corresponding set of fundamental weights, $\boldsymbol{\alpha}_a\cdot\boldsymbol{\omega}_b=\delta_{ab}$.

Key to defining the theories is the notation of the Weyl group of $\mathfrak{g}$, the group generated by reflections in the simple roots:

$$R_a(\boldsymbol{\alpha})=\boldsymbol{\alpha}-\frac{2\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}_a}{\boldsymbol{\alpha}_a^2}\boldsymbol{\alpha}_a \qquad [34]$$

The element $w=R_1R_2\cdots R_r$ is known as a Coxeter element of the Weyl group, and it has special properties that are significant in the present context. In particular, its eigenvalues are of the form $\exp(2\pi\mathrm{i}s_a/h)$, where h is the Coxeter number of $\mathfrak{g}$ and the integers s_a are the exponents of the algebra as in [8]. Note that there is always a pair with $s_1=1$ and $s_r=h-1$. Clearly, w acts as a rotation in the two-dimensional space spanned by the two corresponding eigenvectors. We can define an antisymmetric function $u(\boldsymbol{\alpha},\boldsymbol{\beta})$ on roots to be h/π times the (signed) angle between the projections of $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ onto this two-dimensional eigenspace. In preparation for what follows, it is useful to also define the roots

$$\boldsymbol{\phi}_a=R_rR_{r-1}\cdots R_{a+1}(\boldsymbol{\alpha}_a) \qquad [35]$$

We can now present P Dorey's amazingly compact formula for the complete S-matrix. For the scattering of particle a with particle b,

$$S_{ab}(\theta)=\prod_{\boldsymbol{\beta}\in\Gamma_b}\{1+u(\boldsymbol{\phi}_a,\boldsymbol{\beta})\}^{\boldsymbol{\omega}_a\cdot\boldsymbol{\beta}} \qquad [36]$$

In this formula Γ_b is the set of positive roots of $\mathfrak{g}$ which lie in the orbit of $\boldsymbol{\phi}_b$ under w. We have also defined the building block

$$\{x\}=(x+1)(x-1)$$
$$(x)=\frac{\sinh\left(\dfrac{\theta}{2}+\dfrac{\mathrm{i}\pi x}{h}\right)}{\sinh\left(\dfrac{\theta}{2}-\dfrac{\mathrm{i}\pi x}{h}\right)} \qquad [37]$$

The fusing rules are also particularly elegant in the language of root systems. There is a three-point coupling between $a_i, i=1,2,3$, if there exist three roots $\boldsymbol{\alpha}^{(i)}\in\Gamma_{a_i}$ such that $\boldsymbol{\alpha}^{(1)}+\boldsymbol{\alpha}^{(2)}+\boldsymbol{\alpha}^{(3)}=0$. Furthermore, the fusing occurs in the a_1,a_2 channel at rapidity difference

$$\mathrm{i}u_{a_1a_2}^{\bar{a}_3}=\frac{\mathrm{i}\pi}{h}u(\boldsymbol{\alpha}^{(1)},\boldsymbol{\alpha}^{(2)}) \qquad [38]$$

This is Dorey's fusing rule.

For the case of A_{n-1}, the S-matrices are particularly simple. The mass spectrum is

$$m_a=m\sin\frac{\pi a}{n}, \quad a=1,\ldots,n-1 \qquad [39]$$

and Dorey's rule gives the possible fusings as $ab\to(a+b)\mathrm{mod}\ n$, which occur at the rapidity values

$$\theta=\mathrm{i}u_{ab}=\begin{cases}\mathrm{i}\dfrac{a+b}{n}\pi & a+b<n\\ \mathrm{i}\left(2-\dfrac{a+b}{n}\right)\pi & a+b\geq n\end{cases} \qquad [40]$$

The charge conjugation operator maps $a\to\bar{a}=n-a$ and the explicit form for the S-matrix elements is

$$S_{ab}(\theta)=\{a+b-1\}\{a+b-3\}\cdots\{|a-b|+1\} \qquad [41]$$

The element $S_{ab}(\theta)$ has one direct channel pole at $\theta=\mathrm{i}u_{ab}$ corresponding to the exchange of the particle $a+b$ mod n, and a cross-channel pole at $\theta=\mathrm{i}u_{a\bar{b}}$ corresponding to the exchange of particle $a-b$ mod n.

Affine Toda Theories

The bootstrap program has been solved for all the affine Toda theories. For the simply laced theories described earlier, the result is directly related to the minimal S-matrices constructed above. The only difference is that there are additional factors which depend on the coupling β of the Toda theory but which do not introduce any additional poles onto the physical strip. These CDD factors are included by simply changing the basic building block [37]:

$$\{x\}\to\{x\}_{\mathrm{Toda}}=\frac{(x+1)(x-1)}{(x-1+B)(x+1-B)} \qquad [42]$$

where

$$B=\frac{1}{2\pi}\cdot\frac{\beta^2}{1+\beta^2/4\pi} \qquad [43]$$

The S-matrix structure for the Toda theories based on the nonsimply laced algebras is a good deal more complicated. Integrability is only maintained in the quantum theory if the ratios of the physical masses of the particles depend on the coupling constant β is some very special way.

The Sine-Gordon Theory

We have seen that the sine-Gordon theory has solitons at the classical level. At the quantum level,

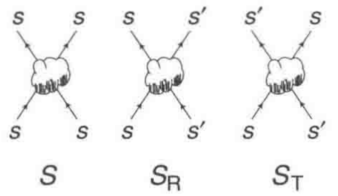


Figure 6 Soliton scattering processes. *s* and *s*′ are the kink and antikink, respectively, or vice versa.

we expect that these kinks become *bona fide* particle states, in addition to the particle corresponding to the quantum fluctuations of the field ϕ. Focusing on the solitons, we expect a degenerate doublet corresponding to the kink and antikink. For the scattering of two solitons, there are six allowed processes illustrated in **Figure 6**. Unitarity [26] leads to the constraints

$$\begin{aligned} &S(\theta)S(-\theta) = 1 \\ &S_{\mathrm{T}}(\theta)S_{T}(-\theta) + S_{\mathrm{R}}(\theta)S_{\mathrm{R}}(-\theta) = 1 \\ &S_{\mathrm{T}}(\theta)S_{\mathrm{R}}(-\theta) + S_{\mathrm{R}}(\theta)S_{\mathrm{T}}(-\theta) = 0 \end{aligned} \qquad [44]$$

while crossing symmetry [27] (using the fact that the soliton and antisoliton are antiparticles) gives

$$S(\mathrm{i}\pi-\theta) = S_T(\theta), \qquad S_{\mathrm{R}}(\mathrm{i}\pi-\theta) = S_R(\theta) \qquad [45]$$

By themselves, these constraints are rather mild; however, the complete soliton *S*-matrix must also satisfy the Yang–Baxter equation [25]. The solution to all the constraints is not unique, however, the Zamolodchikovs conjectured that the exact answer is

$$\begin{aligned} S(\theta) &= \frac{1}{\mathrm{i}\pi}\sinh\left(\frac{8\pi}{\gamma}(\mathrm{i}\pi-\theta)\right)U(\theta) \\ S_{\mathrm{T}}(\theta) &= \frac{1}{\mathrm{i}\pi}\sinh\left(\frac{8\pi}{\gamma}\theta\right)U(\theta) \\ S_{\mathrm{R}}(\theta) &= \frac{1}{\pi}\sin\left(\frac{8\pi^2}{\gamma}\right)U(\theta) \end{aligned} \qquad [46]$$

with

$$\begin{aligned} U(\theta) &= \Gamma\left(\frac{8\pi}{\gamma}\right)\Gamma\left(1+\mathrm{i}\frac{8\theta}{\gamma}\right)\Gamma\left(1-\frac{8\pi}{\gamma}-\mathrm{i}\frac{8\theta}{\gamma}\right) \\ &\quad\times\prod_{n=1}^{\infty}\frac{R_n(\theta)R(\mathrm{i}\pi-\theta)}{R_n(0)R_n(\mathrm{i}\pi)} \\ R_n(\theta) &= \frac{\Gamma\left(2n\frac{8\pi}{\gamma}+\mathrm{i}\frac{8\theta}{\gamma}\right)}{\Gamma\left((2n+1)\frac{8\pi}{\gamma}+\mathrm{i}\frac{8\theta}{\gamma}\right)} \\ &\quad\times\frac{\Gamma\left(1+2n\frac{8\pi}{\gamma}+\mathrm{i}\frac{8\theta}{\gamma}\right)}{\Gamma\left(1+(2n-1)\frac{8\pi}{\gamma}+\mathrm{i}\frac{8\theta}{\gamma}\right)} \end{aligned} \qquad [47]$$

where $\gamma = \beta^2(1-\beta^2/8\pi)^{-1}$. The reason for confidence in the conjecture is that from the soliton *S*-matrix one can complete the bootstrap program and account for all the poles in terms of particles in the theory. In particular, there is a finite set of bound states of the soliton and antisoliton, called breathers, with masses

$$m_k = 2M\sin\frac{k\gamma}{16}, \quad k = 1,2,\ldots < \frac{8\pi}{\gamma} \qquad [48]$$

Here, M is the soliton mass. The bootstrap equations give the *S*-matrix for the scattering of a soliton or antisoliton with the kth breather,

$$\begin{aligned} S_k(\theta) &= \frac{\sinh\theta+\mathrm{i}\cos\frac{k\gamma}{16}}{\sinh\theta-\mathrm{i}\cos\frac{k\gamma}{16}} \\ &\quad\times\prod_{j=1}^{k-1}\frac{\sin^2\left(\frac{k-2j}{32}\gamma-\frac{\pi}{4}+\mathrm{i}\frac{\theta}{2}\right)}{\sin^2\left(\frac{k-2j}{32}\gamma-\frac{\pi}{4}-\mathrm{i}\frac{\theta}{2}\right)} \end{aligned} \qquad [49]$$

while, for the scattering of breather k with l,

$$\begin{aligned} S_{kl}(\theta) &= \frac{\sinh^2\theta+\mathrm{i}\sin\left(\frac{k+l}{16}\gamma\right)\sinh\theta+\mathrm{i}\sin\left(\frac{k-l}{16}\gamma\right)}{\sinh^2\theta-\mathrm{i}\sin\left(\frac{k+l}{16}\gamma\right)\sinh\theta-\mathrm{i}\sin\left(\frac{k-l}{16}\gamma\right)} \\ &\quad\times\prod_{j=1}^{l-1}\frac{\sin^2\left(\frac{k-l-2j}{32}\gamma+\mathrm{i}\frac{\theta}{2}\right)\cos^2\left(\frac{k+l-2j}{32}\gamma+\mathrm{i}\frac{\theta}{2}\right)}{\sin^2\left(\frac{k-l-2j}{32}\gamma-\mathrm{i}\frac{\theta}{2}\right)\cos^2\left(\frac{k+l-2j}{32}\gamma-\mathrm{i}\frac{\theta}{2}\right)} \end{aligned} \qquad [50]$$

where we assume, without loss of generality, that $k \geq l$. The remarkable thing is that the scattering of the lowest-mass breather m_1 with itself,

$$S_{11}(\theta) = \frac{\sinh\theta + \mathrm{i}\sin\frac{\gamma}{8}}{\sinh\theta - \mathrm{i}\sin\frac{\gamma}{8}} \qquad [51]$$

is precisely the Toda S-matrix for A_1 with $\beta \to \mathrm{i}\beta/\sqrt{2}$ (the origin of the factor of $\sqrt{2}$ is mentioned after eqn [9]). This uniquely identifies the lowest-mass breather as being the quantum of the ϕ field.

The quantum structure that we have described above can be directly related to the classical scattering of solitons. In order to implement the classical limit, we can reintroduce $\hbar$ which is achieved by replacing β^2 by $\beta^2\hbar$. In this limit, the S-matrix elements have the form

$$S(\theta) = \exp\frac{2\mathrm{i}}{\hbar}(\delta(\theta) + \mathcal{O}(\hbar)) \qquad [52]$$

The phase $\delta(\theta)$ is related via the WKB approximation to the time delay in the classical theory of soliton scattering via

$$\delta(\theta) = \text{const.} + \int_0^\theta \mathrm{d}\theta' M \sinh(\theta/2)\Delta t(\theta) \qquad [53]$$

where $\Delta t(\theta)$ is the time delay in the center of mass (21). It is possible to verify [53] for the processes $S(\theta)$ and $S_{\mathrm{T}}(\theta)$. Note that the reflection process has no classical analogue.

IQFT, Conformal Field Theories and Statistical Systems

We have described some IQFTs and their factorizable S-matrices in theories with a mass gap. We can ask the question, "what happens at very high energies compared with all the mass scales?" For a generic QFT such a limit may not exist, however, for a special class of theories the limit is a massless scale-invariant theory corresponding to a fixed point of the renormalization group. The massive theory can be thought of as a deformation of the massless theory by a particular relevant operator. At the fixed point, the Poincaré symmetry is enhanced to the full conformal group in the appropriate number of dimensions and the resulting theory is known as a conformal field theory (CFT). In $1+1$ dimensions the conformal group is infinite dimensional and so many CFTs are themselves integrable, in the sense that the complete spectrum of fields is known and their correlation functions can be constructed. Hence, an alternative way of thinking about many IQFTs is as a perturbation of a CFT by a specific relevant operator:

$$S_{\mathrm{IQFT}} = S_{\mathrm{CFT}} + g\int \mathrm{d}^2x\,\mathcal{O}(x) \qquad [54]$$

We will suppose that the operator has conformal dimensions $(\Delta, \bar{\Delta})$. This description of the theory can be turned around to ask the following question: which relevant deformations of a given CFT lead to IQFTs? Remarkably, since CFTs are so well understood, the question can often be answered exactly. The idea is that the conserved quantities of a CFT are all (anti-)holomorphic with respect to a holomorphic coordinate $z = x + \mathrm{i}t$. Conserved quantities include the stress tensor of spin 2 but include, in addition, an infinite tower of currents of ever increasing spin $\{T_s\}$. After perturbation, one has

$$\bar{\partial}T_s = gR^{(1)} + \cdots + g^n R^{(n)} + \cdots \qquad [55]$$

The conformal dimensions of the $R^{(n)}$ are $(s - n(1-\Delta), 1 - n(1-\Delta))$. Since the conformal dimensions of fields in a CFT are bounded below by zero, it follows that the series on the right-hand side truncates. The question of whether T_s remains conserved away from the CFT boils down to the question as to whether the right-hand side has the form $\partial\Theta$, for some Θ. Zamolodchikov found an ingenious counting argument which showed in certain circumstances that the right-hand side has precisely this form for some $s > 2$. This is sufficient to establish that the perturbed theory is an IQFT. In certain cases the spectrum of spins of the conserved quantities that are established by the counting argument is enough to make a connection with a known factorizable S-matrix.

This way of viewing IQFT as perturbations of CFTs is especially fruitful when we make the connection of the Euclidean QFT with the classical statistical mechanics of a two-dimensional system. In this connection, the Feynman path integral is reinterpreted as the sum over the configurations in the canonical ensemble with the Euclidean action interpreted as the energy. Usually, we consider statistical systems which are discrete, so typically defined on a lattice. The Euclidean QFTs are to be thought of as these statistical systems in the continuum limit where the lattice spacing is taken to zero keeping the long-range physics fixed. CFTs which have no massive degrees of freedom are identified with points of second-order phase transitions in the statistical system where correlation lengths are infinite. Perturbations of CFTs by relevant operators correspond to taking the statistical system away from criticality by changing some external parameter.

The prototypical example of such a statistical system is the Ising model. In the lattice version of

this model, there are a set spins $\{\sigma_i\}$ at each lattice site which can take the discrete values ± 1. The partition function of the theory is

$$Z(H,T) = \sum_{\{\sigma_i\}} \exp\left(-T^{-1}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - H\sum_i \sigma_i\right) \quad [56]$$

The Ising model is the simplest model of a ferromagnet, where T is the temperature and H is the external applied field. The theory has a second-order phase transition for $T = T_c$, the Curie temperature, and $H = 0$ when the competition between the energy, which favors aligning the spins, and entropy, which favors disorder, exactly balance. In the two-dimensional neighborhood of the critical point, the lattice theory admits a continuum limit which can be described as the perturbation of a CFT, describing the critical Ising model, by a pair of relevant operators with couplings $T - T_c$ and H. In the case of the Ising model, the CFT is simply the theory of a free massless fermion in two-dimensional Euclidean space.

It turns out that in the two-dimensional space of relevant perturbations, there are two directions which lead to IQFTs. The most obvious is changing the temperature away from T_c while keeping $H = 0$. This leads to a particularly simple IQFT, that of a free massive fermion. More unexpectedly, the direction for which H varies away from 0, but $T = T_c$, also leads to an IQFT. In this case, Zamolodchikov's counting argument shows that there are higher-spin conserved charges of spin including

$$s = 1, 7, 11, 13, 17, 19, \ldots \quad [57]$$

This is remarkable because, as we have described previously, there is a minimal solution of the bootstrap program that describes the scattering of eight particles which has a spectrum of conserved charges that includes these spins. It is the minimal scattering theory related to the algebra E_8.

The fact that the scattering theory of the off-critical Ising model in the magnetic field direction has been identified is remarkable. From the S-matrix one can proceed to investigate the off-critical correlation functions using a technique known as the "form factor programe." Detailed simulation of the original lattice model [56] has provided strong support for the veracity of the E_8 scattering theory. For instance, the two lightest masses in the scattering theory determine the ratio of the two longest correlation lengths $m_2/m_1 = 2\cos(\pi/5)$.

In general, the identification of an IQFT and the CFT at its ultraviolet limit can be more difficult to establish. One way to proceed is to use the thermodynamic Bethe ansatz. This technique involves considering the thermodynamics of a gas of the particles in a periodic box. Since the scattering is purely elastic, thermodynamic quantities can be calculated, albeit in terms of a set of coupled nonlinear integral equations. If the box is small enough, ultraviolet effects dominate and various features of the CFT can be recovered.

Other IQFTs

There is a rich menagerie of other IQFTs that we have no space to discuss in detail. One is sigma models, whose fields take values in a Riemannian target space $\mathfrak{M}$ with an action

$$S = \int d^2x g_{ab}\partial_\mu X^a \partial^\mu X^b \quad [58]$$

where $g_{ab}dX^a\, dX^b$ is the metric of $\mathfrak{M}$. These theories are integrable at the classical level if the target space is either a group manifold of a compact simple group G or a symmetric space coset G/H, where H is a suitable subgroup of G. The former are known as the "principal chiral models." There are two kinds of conserved quantities, both local and nonlocal. At the quantum level, the conserved currents which imply classical integrability can be subject to quantum anomalies. An analysis of these anomalies proves that the principal chiral models are all integrable at the quantum level, while only the subset of symmetric space coset models, namely

$$\begin{gathered} SO(n+1)/SO(n), \qquad SU(n)/SO(n) \\ SU(2n)/Sp(n), \qquad SO(2n)/SO(n)\times SO(n) \\ Sp(2n)/Sp(n)\times Sp(n) \end{gathered} \quad [59]$$

are quantum integrable. S-matrices have been proposed for all these integrable sigma models. They have a more complicated structure than most of the cases discussed here, because the particles fall into representations of the associated Lie groups and the Yang–Baxter equation, such as for the sine-Gordon solitons, is now nontrivial. Remarkably, gross features of the S-matrices, such as the mass spectrum fusing rules, are identical to the Toda theories or the minimal S-matrices.

Returning to IQFTs that are associated with deformations of CFTs, there are more general classes which are associated with the renormalization group trajectories between two nontrivial fixed points. These theories have both massless and massive degrees of freedom. Even more remarkable are the staircase models of Zamolodchikov that exhibit an infinite series of crossover behavior where the renormalization group trajectory passes close to an infinite series of fixed points in sequence.

For all of the theories described above, one might have thought more generally that integrability is a very rigid property of a theory. In general, for example, the number of external coupling constants is very limited and the mass ratios are all fixed. For

example, in Toda theories there is only an overall mass scale m and the coupling β. If the form of the potential is altered in any way then integrability is lost. However, in certain circumstances, integrability appears to be a looser constraint that allows more flexibility. One class of such theories is known as the homogeneous sine-Gordon theories. These are integrable deformations of gauged WZW models associated with the coset $G/U(1)^r$, where r is the rank of a simple compact group G. In these theories there is a rich spectrum of both stable and unstable particles with masses and an S-matrix that depends continuously on a set of r coupling constants.

See also: Algebraic Approach to Quantum Field Theory; Bethe Ansatz; Constructive Quantum Field Theory; Eight Vertex and Hard Hexagon Models; Functional Equations and Integrable Systems; Integrable Systems: Overview; Quantum Field Theory: A Brief Introduction; Quantum Field Theory in Curved Spacetime; Sine-Gordon Equation; Symmetries in Quantum Field Theory of Lower Spacetime Dimensions; Two-Dimensional Models; Yang–Baxter Equations.

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Integrable Discrete Systems

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Discrete Dynamical Systems

The expression "dynamical system" usually refers to a coupled system of ordinary differential equations (ODEs), namely,

$$\dot{x}_j(t) = f_j(t, x_1, \ldots, x_N), \quad j = 1, \ldots, N \qquad [1]$$

where t belongs to some set of nonzero measure I of the real line $\mathbb{R}$, typically an interval $[a, b]$ or a semiline or the whole line, and x_j are sufficiently smooth functions from I to $\mathbb{R}$ or to $\mathbb{C}$.

The system [1] is complemented by initial or boundary conditions that make it into an "initial-value" or a "boundary-value" problem. Under suitable regularity assumptions on the RHS, the existence and uniqueness of the solution of the initial-value problem is guaranteed, but in most cases the solution can be known only "approximately" either through perturbation theory or just through numerical integration. This is not the proper place to discuss finite-difference schemes for systems of ODEs: what is relevant is that such numerical schemes (think, e.g., of Euler or Runge–Kutta schemes) "discretize" the continuous independent variable t by replacing it by an integer variable $n \in \mathbb{Z}$: in the simplest case, the interval $[a, b]$ is replaced by a set of L equally spaced points $t_n = a + n(b-a)/L (n = 1, \ldots, L)$, the first derivative is approximated by a (forward) difference, and the system [1] is converted into a system of "difference" equations of the form

$$x_j(n+1) = x_j(n) + hF(n, x_1(n), \ldots, x_N(n)) \qquad [2]$$

where h denotes the time step $(b-a)/L$.

The coupled system [2] is an example of a "discrete dynamical system," explicit (because the updated variables only depend upon the values taken

at previous discrete times), first order (only "nearest-neighbor" discrete times, $n, n+1$ are involved), but nonautonomous, as the RHS is allowed to depend explicitly upon the independent variable n, analogously to its continuum counterpart.

In the following, "autonomous" but not necessarily explicit discrete dynamical systems of a special type will be considered: in fact, we will require them to be equipped with a Hamiltonian structure, and we will define the notion of complete integrability (in the Arnol'd–Liouville sense) for such systems.

This article emphasizes on some aspects and properties of integrable discrete systems, neglecting others that could be equally important. In particular, as no nonautonomous discrete systems will be considered, discrete analogs of Painleve' equations will never be discussed in this article, and consequently the intriguing issues concerning "singularity confinement" in the discrete and "algebraic entropy" will not be touched upon (see, e.g., Grammaticos *et al.* (2004)). Similarly, neither the integrability for discrete systems in multidimensional space nor "quantum integrable mappings" will be discussed.

Lagrangian and Hamiltonian Formulations

Following the historical path along which modern classical mechanics has been developed, first the concept of a Lagrangian map is introduced, and then Hamiltonian (in fact, symplectic) maps are defined through a proper discrete version of the Legendre transformation.

Let $x_j(n)$ $(j=1,\ldots,N, n\in\mathbb{Z})$ be N sequences of real numbers and let $\mathcal{L}(\boldsymbol{x},\boldsymbol{y})$ be a smooth function from $\mathbb{R}^N\times\mathbb{R}^N$ into the reals, $\boldsymbol{x}$ denoting the N-tuple $x_1,\ldots,x_N$. $\mathcal{L}$ is regarded as a "discrete Lagrange function": corresponding to each discrete time n, it is assigned a certain value $\mathcal{L}_n := \mathcal{L}(\boldsymbol{x}(n),\boldsymbol{x}(n+1))$. The corresponding discrete action functional $S[\mathcal{L}]$ is defined in a natural way:

$$S[\mathcal{L}] = \sum_{n=N_a}^{N_b} \mathcal{L}_n \qquad [3]$$

The actual "discrete trajectory" will be given by the sequence $\boldsymbol{x}(n)$ that corresponds to a "critical point" of the action [3] subject to the constraints $\delta\boldsymbol{x}(N_a)=\delta\boldsymbol{x}(N_b)=0$. Note that the values $N_a\,(N_b)$ may well possibly coincide with $-\infty\,(+\infty)$. Such "critical points" are given by the solution of the discrete Euler–Lagrange equations:

$$\left.\frac{\partial\mathcal{L}}{\partial x_j}\right|_{x_j=x_j(n),y_j=x_j(n+1)} + \left.\frac{\partial\mathcal{L}}{\partial y_j}\right|_{x_j=x_j(n-1),y_j=x_j(n)} = 0 \qquad [4]$$

It is worthwhile to remark the intrinsic nature of eqns [4], whose form turns out to be independent of the choice of a coordinate chart. In fact, by omitting the explicit dependence on n and simply denoting $\boldsymbol{x}(n)=\boldsymbol{x}$, $\boldsymbol{x}(n+1)=\tilde{\boldsymbol{x}}$, $\boldsymbol{x}(n-1)=\underset{\sim}{\boldsymbol{x}}$, [4] can be cast in the form

$$\nabla_1\mathcal{L}(\boldsymbol{x},\tilde{\boldsymbol{x}}) + \nabla_2\mathcal{L}(\underset{\sim}{\boldsymbol{x}},\boldsymbol{x}) = 0 \qquad [5]$$

which makes its "implicit" nature for the updated variable $\tilde{\boldsymbol{x}}$ more transparent. Clearly, as a map from the pair $(\underset{\sim}{\boldsymbol{x}},\boldsymbol{x})$ to the pair $(\boldsymbol{x},\tilde{\boldsymbol{x}})$, it is in general a multivalued map, or a "correspondence", as it is called in the literature (Suris 2003, Veselov 1991). In order that [5] be solvable for $\tilde{\boldsymbol{x}}$, the Hessian matrix $H_{jk}=\partial^2\mathcal{L}/\partial x_j\partial y_k$ should be nondegenerate.

As will be noted shortly, the Lagrangian map [4] (or [5]) is in fact a canonical, or better a symplectic transformation on a suitably defined cotangent bundle T^*X to the configuration space $X\in\mathbb{R}^N$. Namely, one defines the conjugate momentum to $\boldsymbol{x}$ as

$$\boldsymbol{p} := \nabla_2\mathcal{L}(\underset{\sim}{\boldsymbol{x}},\boldsymbol{x}) \qquad [6]$$

so that [5] can be rewritten as the following system:

$$\boldsymbol{p} = -\nabla_1\mathcal{L}(\boldsymbol{x},\tilde{\boldsymbol{x}}) \qquad [7]$$

$$\tilde{\boldsymbol{p}} = \nabla_2\mathcal{L}(\boldsymbol{x},\tilde{\boldsymbol{x}}) \qquad [8]$$

This system defines a correspondence $(\boldsymbol{x},\boldsymbol{p})\to(\tilde{\boldsymbol{x}},\tilde{\boldsymbol{p}})$, which is indeed a "symplectic" one, as it preserves the standard symplectic form $\omega(\boldsymbol{x},\boldsymbol{p})=\sum_{j=1}^N \mathrm{d}p_j\wedge \mathrm{d}x_j$, and, of course, the associated Poisson brackets. The simplest way to recognize this property is by constructing the generating function of the corresponding canonical transformation. To this end, let us introduce

$$\mathcal{S}(\boldsymbol{x},\tilde{\boldsymbol{p}}) = -\mathcal{L} + \sum_{j=1}^N \tilde{p}_j(\tilde{x}_j - x_j) \qquad [9]$$

The discrete Euler–Lagrange equation then takes the form

$$\tilde{x}_j - x_j = \frac{\partial\mathcal{S}}{\partial\tilde{p}_j} \qquad [10]$$

$$p_j - \tilde{p}_j = \frac{\partial\mathcal{S}}{\partial x_j} \qquad [11]$$

which is canonically generated by $\mathcal{S}+\sum_j x(j)\tilde{p}(j)$. A strict analog of the Hamiltonian formulation for continuous-time Lagrangian systems does not indeed exist in the discrete-time case. One of the main consequences, well known to the specialists but worth emphasizing in the present context, is that even a symplectic map in one degree of freedom

(two-dimensional T^*X) is generically not integrable: the existence of an invariant function $F(x,p) = F(\tilde{x},\tilde{p})$ is not entailed by the symplectic structure, so that, as discussed later, integrable maps of the standard type are indeed exceptional. On the other hand, note that invariant functions do exist whenever a Lagrangian has some additional symmetry: this is the case when a Lie group acts on the configuration space X and the Lagrange function is invariant under its induced action on $X \times X$, so that a discrete version of the Noether theorem applies (Suris 2003).

Complete Integrability

The definition of a "completely integrable" discrete-time system is now in order. Let Φ be a symplectic map on the $2N$-dimensional phase space $\mathcal{M} := (\mathbb{R}^{2N}, dp \wedge dq)$, equipped with N smooth invariant functions F_j, such that

- $F_1, \ldots, F_N$ are functionally independent, that is, their gradients ∇F_j are linearly independent of $\mathcal{M}$;
- $F_1, \ldots, F_N$ are in involution:

$$\{F_j, F_k\} = 0, \quad j,k = 1, \ldots, N$$

Let $\mathcal{T}$ be a connected component of the common level set

$$\{(x,p) \in \mathcal{T}:\ F_k(x,p) = c_k,\ k = 1, \ldots, N\}$$

Then $\mathcal{T}$ is diffeomorphic to $\mathbb{T}^l \times \mathbb{R}^{N-l}$, for some $0 \leq l \leq N$; if $\mathcal{T}$ is compact, then it is diffeomorphic to an N-dimensional torus $\mathbb{T}^N$.

In the compact case, there exists an open ball $\Omega \in \mathbb{R}^N$ such that, in $\mathcal{T} \times \Omega$, there exist new canonical coordinates $(I_k, \phi_k), k = 1, \ldots, N$; $I_k \in \mathcal{T}, \phi_k \in \Omega$, the so-called action-angle coordinates, enjoying the following properties:

- the actions I_k depend just on the F_j's
- in action-angle coordinates the map is a linear shift on the N-dimensional torus:

$$\tilde{I}_k := \Phi(I_k) = I_k$$
$$\tilde{\phi}_k := \Phi(\phi_k) = \phi_k + \nu_k(I_1, I_2, \ldots, I_N)$$

Hence, in action-angle variables a completely integrable map is a canonical transformation from (I, ϕ) to $(\tilde{I}(=I), \tilde{\phi})$, whose generating function W only depends on the action variables. It takes the form

$$\tilde{I}_k - I_k = 0 \qquad [12]$$

$$\tilde{\phi}_k - \phi_k = \frac{\partial W}{\partial I_k} := \frac{\partial}{\partial I_k} \sum_{j=1}^{N} \int_x^{\tilde{x}} dx_j\ p_j(I,x) \qquad [13]$$

Integrable Maps of the Standard Type

As the simplest integrable models, first consider some highly nontrivial examples of "standard maps," that is, scalar discrete second-order difference equations of the following type (Suris 2003):

$$x_{n+1} - 2x_n + x_{n-1} = G(x_n; h) \qquad [14]$$

with h a real parameter, which exhibit an invariant function, say

$$J(x_{n-1}, x_n) = J(x_n, x_n + 1) \qquad [15]$$

Clearly, [14] can serve as a discretization of the Newtonian equation:

$$\ddot{x} = f(x) \qquad [16]$$

if $\lim_{h \to 0} h^2 G(x; h)$ exists and is equal to $f(x)$.

All "standard maps" are Lagrangian, being stationary points of the discrete action:

$$S = \sum_{n \in \mathbb{Z}} \left(\tfrac{1}{2} [x_{n+1} - x_n]^2 + V(x_n; h) \right) \qquad [17]$$

with $G(x; h) = \partial V(x; h)/\partial x$. A point in the phase space is a pair $x_n, p_n = x_n - x_{n-1}$, and [14] is symplectic for $dp \wedge dx$, reading

$$x_{n+1} - x_n = p_{n+1} \qquad [18]$$

$$p_n - p_{n+1} = G(x_n; h) \qquad [19]$$

The corresponding generating function is given by $S = V(x; h) + (1/2)p_{n+1}^2$. Integrability of [19] means the existence of a function F from $\mathcal{M}$ into itself such that

$$F(x_{n+1}, p_{n+1}) = F(x_n, p_n) \qquad [20]$$

where [15] and [20] are equivalent provided $J(x, x - y) = F(x, y)$.

Suris has found three families of functions G that ensure integrability: a rational family, a trigonometric family, and a hyperbolic family. There is no room here to display the relevant formulas, nor to explain why, under natural analiticity assumptions both in h and x, no other integrable family exists. However, it is worth mentioning that they turn out to be integrable discretizations of the scalar second-order differential equations [16] for the following "force" functions $f(x)$:

$$f_{\text{rat}}(x) = A + Bx + Cx^2 + DX^3 \qquad [21]$$

$$f_{\text{trig}}(x) = A\sin(\omega x) + B\cos(\omega x) + C\sin(\omega 2x) + D\cos(\omega 2x) \qquad [22]$$

$$f_{\text{hyp}}(x) = A\exp(x) + B\exp(-x) + C\exp(2x) + D\exp(-2x) \qquad [23]$$

A curious fact is that those Newton forces that one can "discretize" in order to get integrable maps

are exactly the external forces that one can add to the internal two-body interactions of the Calogero–Moser or Calogero–Sutherland models to preserve complete integrability.

Integrable Discrete Systems and the Lax Approach

Since, in a seminal paper, Lax (1968) introduced it for the Korteweg–de Vries (KdV) equation, the search for a "Lax representation" played a crucial role in the construction of integrable systems, both finite and infinite dimensional. In particular, the continuous time dynamical system [1] (assumed to be autonomous) is said to be equipped with a Lax representation if there exist two matrices L, M whose entries depend upon the coordinates x_j, whenceforth upon the time t, such that the time evolution [1] can be cast in the form

$$\dot{L}(t) = [L(t), M(t)] \qquad [24]$$

Hence, the one-parameter family of matrices $L(t)$ undergoes the "isospectral" deformation:

$$L(t) = U(t)L(0)(U(t))^{-1} \qquad [25]$$

$U(t)$ being the unique solution of the linear matrix differential equation:

$$\dot{U}(t) = M(t)U(t) \qquad [26]$$

with the initial condition $U(0) = I$. Then, the existence of a Lax representation in term of, say, $k \times k$ matrices entails the existence of k integrals of motion, given, for instance, by the eigenvalues of $L(t)$, or by the traces $t_l := \mathrm{tr}(L(t))^l$.

Some remarks are in order:

- In the case of a Hamiltonian system, the matrices L, M depend, of course, on the point in the phase space.
- No guarantee exists, *a priori*, that the eigenvalues of L, or equivalently the traces t_l, be "sufficiently many" and in involution. Note, however, that in many examples the Lax matrices L, M depend on an extra scalar parameter λ (so that they are elements of an affine or "loop" Lie algebra), which might increase the number of integrals of motion well beyond the dimension of the matrix.

The N-body systems of Calogero type and Toda type are celebrated examples of integrable dynamical systems equipped with a Lax representation.

How this description can be adapted to the discrete-time case? The isospectral equation [25] suggests the proper way. One has to look for two matrices depending on the coordinates (or on the phase-space variables) $\boldsymbol{x}$ (again, they can be called L, M), such that the discrete-time evolution, modeled, for instance, by [2], can be cast in the form of a similarity transformation:

$$\tilde{L} = MLM^{-1} \qquad [27]$$

where $L = L(\boldsymbol{x})$, $\tilde{L} = L(\tilde{\boldsymbol{x}})$, and $M = M(\boldsymbol{x}, \tilde{\boldsymbol{x}})$. As usual, by denoting by n the discrete time (i.e., the number of iterations), so that $\boldsymbol{x} = \boldsymbol{x}(n), \tilde{\boldsymbol{x}} = \boldsymbol{x}(n+1)$, eqn [27] implies that a discrete version of [25] holds:

$$L(n) = U(n)L(0)[U(n)]^{-1} \qquad [28]$$

where $U(n) := M(n)M(n-1)\cdots M(1)$.

As in the continuous case, the existence of a discrete Lax representation entails the existence of conserved quantities (invariants of the map or of the correspondence) but by itself it does not say anything about completeness and involutivity of such invariants. There is, however, an approach that incorporates the involutivity property in the very construction of Lax equations, both discrete and continuous, namely the "R-matrix approach." Indeed, from the experimental observation of a number of examples, both finite and infinite dimensional, one can assert that the matrix M taking part in the "continuous" Lax representation [24] may be presented in the form (Suris 2003)

$$M = R(f(L)) \qquad [29]$$

In [29], L, M are element of some matrix Lie algebra $\boldsymbol{g}$, R is a linear map from $\boldsymbol{g}$ into itself, and f is a conjugation-covariant function, namely

$$f(ALA^{-1}) = Af(L)A^{-1} \qquad [30]$$

A being an arbitrary element of the group $\boldsymbol{G}$ with Lie algebra $\boldsymbol{g}$.

Polynomials in the variable L with scalar coefficients are typical examples of conjugation-covariant functions. Moreover, in a matrix Lie algebra, one can identify $\boldsymbol{g}$ with its dual space $\boldsymbol{g}^*$ through the nondegenerate bilinear form provided by the trace: $(L_1, L_2) := \mathrm{tr}(L_1 L_2)$. Then, the trace F of a conjugation-covariant function f will be a typical example of a conjugation-invariant function, and, conversely, the gradient of a conjugation-invariant function F, defined as

$$\langle \nabla F, X \rangle = \frac{\mathrm{d}}{\mathrm{d}\epsilon} F(L + \epsilon X)|_{\epsilon=0} \qquad [31]$$

will be a typical example of a conjugation-covariant function. In the above setting, one can define the following Lie–Poisson bracket on $\boldsymbol{g}$:

$$\{F, G\}(L) := (L, [\nabla F, \nabla G]) \qquad [32]$$

where F, G are arbitrary (i.e., not necessarily invariant) functions from $\mathbf{g}$ into $\mathbb{C}$, so that the Hamilton equation

$$\dot{L} = \{H, L\} \qquad [33]$$

takes the Lax form

$$\dot{L} = [L, \nabla H] \qquad [34]$$

It is immediate to check that invariant functions of L are Casimir functions of [32] so that they will not generate any nontrivial flow.

Assume now that the linear mapping R, usually called r-matrix, introduced in [29], is such that it defines a new Lie bracket on $\mathbf{g}$, through the formula

$$[L_1, L_2]_R = \tfrac{1}{2}([L_1, R(L_2)] + [R(L_1), L_2]) \qquad [35]$$

and consequently a new Lie–Poisson bracket

$$\{F, G\}_R(L) := (L, [\nabla F, \nabla G]_R) \qquad [36]$$

Then the following theorem holds:

Let H be an invariant function on $\mathbf{g}$. *Then*:

(i) *The Hamilton equations on* $\mathbf{g}$ *generated by H with respect to the Poisson bracket* [36] *have the Lax form*

$$\dot{L} = [L, R(\nabla H)] \qquad [37]$$

(ii) *The invariants of* $\mathbf{g}$, *that is, the Casimir function of the standard Lie–Poisson bracket* [32], *are in involution for* [36] *so that the corresponding flows are mutually commuting.*

A particular realization of such R operator, very important for the application, arises in the so-called Adler–Kostant–Symes (AKS) construction (Adler 1979, Kostant 1979, Symes 1980), where the Lie algebra $\mathbf{g}$ admits a decomposition in two subalgebras, $\mathbf{g}_+$ and $\mathbf{g}_-$, so that, as linear spaces, it holds that

$$\mathbf{g} = \mathbf{g}_+ \oplus \mathbf{g}_- \qquad [38]$$

Denoting by $\pi_\pm$ the corresponding projections, the linear mapping

$$R := \pi_+ - \pi_- \qquad [39]$$

defines a new Lie bracket on $\mathbf{g}$, and the corresponding Lax equations take the two equivalent forms:

$$\dot{L} = [L, \pi_+(f(L))] = -[L, \pi_-(f(L))] \qquad [40]$$

For the present purposes, it is of paramount importance that the AKS construction has a discrete-time version (Suris 2003).

In fact, let $\mathbf{G}$ be a Lie group with Lie algebra $\mathbf{g}$, and let $\mathbf{G}_+, \mathbf{G}_-$ be its subgroups having $\mathbf{g}_+, \mathbf{g}_-$ as Lie algebras. Then, in a certain component of the identity element I, any element g of $\mathbf{G}$ is uniquely factorizable as

$$g = \Pi_+(g)\Pi_-(g), \quad \Pi_\pm(g) \in \mathbf{G}_\pm \qquad [41]$$

Moreover, let $F: \mathbf{g} \to \mathbf{G}$ be a conjugation-covariant function. Consider now the map

$$\begin{aligned} L \to \tilde{L} &:= \Pi_+^{-1}(F(L)) \cdot L \cdot \Pi_+(F(L)) \\ &= \Pi_-(F(L)) \cdot L \cdot \Pi_-^{-1}(F(L)) \end{aligned} \qquad [42]$$

and regard it as a difference equation, yielding $\tilde{L} = L(n+1)$ in terms of $L = L(n)$. Then, the following properties hold:

- For whatever function F, the map [42] commutes with any continuous flow [40], mapping solutions into solutions.
- It can be "explicitly integrated" with respect to the discrete time n, yielding

  $$L(n) = \Pi_+^{-1}(F^n(L_0)) \cdot L_0 \cdot \Pi_+(F^n(L_0)) \qquad [43]$$

  or the equivalent expression in terms of the complementary projection Π_-.
- It is interpolated by the continuous flow [40] with time step h if

  $$\exp(hf(L)) = F(L) \leftrightarrow f(L) = h^{-1} \log(F(L)) \qquad [44]$$

  In other words, the discrete-time systems that one derives through this approach are just a sequence of pictures taken at equally spaced times of some continuous flow pertaining to the hierarchy [40]: so, by construction they are Poisson maps with an involutive family of integrals given by the conjugation-invariant functions of L (typically, $\operatorname{tr} L^n$).
- As far as

  $$F(L) = I + hf(L) + o(h^2) \qquad [45]$$

  the map [42] serves as an integrable exact discretization of the flow [40], sharing both its Poisson structure and its constants of the motion.

An Integrable Discretization of the Toda Lattice

Consider a simple but an illuminating example of the above construction, showing an integrable discretization of the "open-end Toda lattice," which is described (Suris 2003) by the Newtonian equations of motion:

$$\begin{aligned} &\ddot{x}_j = \exp(x_{j+1} - x_j) - \exp(x_j - x_{j-1}) \\ &j = 1, \ldots, N \end{aligned} \qquad [46]$$

and can be cast into a Hamiltonian form by setting $p_j = \dot{x}_j$; $q_j = x_j$. If, according to H Flaschka (1974), one introduces the variables

$$b_j = \dot{x}_j, \qquad a_j = \exp(x_{j+1} - x_j) \qquad [47]$$

eqn [46] takes the form

$$\dot{b}_j = a_j - a_{j-1}, \qquad \dot{a}_j = a_j(b_{j+1} - b_j) \qquad [48]$$

and enjoys the Lax representation [24] in terms of the $N \times N$ matrices:

$$L(a,b) = \sum_{k=1}^{N} a_j E_{j,j+1} + \sum_{k=1}^{N} b_j E_{j,j} + \sum_{k=1}^{N} E_{j+1,j} \qquad [49]$$

$$\begin{aligned} M(a,b) &= A := \sum_{k=1}^{N} a_j E_{j,j+1} \quad \text{or} \\ M(a,b) &= -B := \sum_{k=1}^{N} b_j E_{j,j} + \sum_{k=1}^{N} E_{j+1,j} \end{aligned} \qquad [50]$$

In the above formula, $E_{j,k}$ is the matrix having 1 in the jk position and 0 elsewhere, so that, obviously, $E_{N,N+1} = E_{N+1,N} = 0$. An inspection to [49] and [50] shows that A is just the strictly upper triangular part of $L(a,b)$, while B is its lower triangular part. The pair (A, B) constitutes the so-called LU decomposition of $L(a,b)$. One is clearly in the AKS setting, the Lie algebra $\boldsymbol{g}$ being just the algebra of $N \times N$ matrices, and the Lie subalgebras $\boldsymbol{g}_\pm$ being the strictly upper and lower triangular matrices. The tridiagonal matrix $L(a,b)$ belongs to a Poisson submanifold of $\boldsymbol{g}$, invariant under the flows [40], and a complete family of commuting integrals of motion is given, for instance, by $I_k = \mathrm{tr} L^k$.

Now, the elements of the group GL_N, realized as the group of invertible $N \times N$ matrices, uniquely factorize into a product of an invertible lower-triangular matrix times an upper-triangular matrix with units on the diagonal, and the Lie algebras of those subgroups are just the aforementioned subalgebras $\boldsymbol{g}_\pm$. Then, one is naturally tempted to look for an integrable discretization provided by a conjugation-covariant function of the type [45], starting with the simplest possible choice, namely

$$F(L) = I + hf(L)$$

Setting

$$\begin{aligned} \tilde{L}(a,b) &:= L(\tilde{a}, \tilde{b}) \\ &= \Pi_+^{-1}(I + hL) \cdot L \cdot \Pi_+(I + hL) \\ &= \Pi_-(I + hL) \cdot L \cdot \Pi_-^{-1}(1 + hL) \end{aligned} \qquad [51]$$

it turns out that the matrix equation [51] is equivalent to the map

$$(a,b) \to (\tilde{a}, \tilde{b})$$

described by the following equations:

$$\begin{aligned} \tilde{b}_k &= b_k + h\left(\frac{a_k}{\beta_k} - \frac{a_{k-1}}{\beta_{k-1}}\right) \\ \tilde{a}_k &= a_k(\beta_{k+1} - \beta_k) \end{aligned}$$

where β_k, which are the "field variables" entering into the LU factorization [51], are explicitly and uniquely defined by the recurrent relation (amounting to a finite continued fraction):

$$\beta_k = 1 + hb_k - h^2 \frac{a_{k-1}}{\beta_{k-1}}, \qquad k = 1, \ldots, N \qquad [52]$$

As $a_0 = 0$, the initial condition is simply $\beta_1 = 1 + hb_1$.

It follows from the general results of the previous section that [51] is an integrable Poisson map, sharing with the continuous Toda hierarchy both the Poisson structure and the integrals of motion. Its initial-value problem can be uniquely solved in terms of the LU factorization of the group element $(I + hL_0)^n$, the initial condition L_0 being any matrix pertaining to the tridiagonal submanifold [49]. According to [44], the interpolating Hamiltonian flow is provided by the function $f(L) = h^{-1} \log(1 + hL)$. To make contact with the discussion in the section "Lagrangian and Hamiltonian formulations," we observe that, in terms of the canonical variables x_j, p_j, the discrete Toda [51] lattice becomes the following symplectic map:

$$1 + hp_j = \exp(\tilde{x}_j - x_j) + h^2 \exp(x_j - \tilde{x}_{j-1}) \qquad [53]$$

$$1 + h\tilde{p}_j = \exp(\tilde{x}_j - x_j) + h^2 \exp(x_{j+1} - \tilde{x}_j) \qquad [54]$$

It can evidently be written in the discrete Newtonian form:

$$\begin{aligned} &\exp(\tilde{x}_j - x_j) - \exp(x_j - \underset{\sim}{x}_j) \\ &\quad = h^2 \exp(\underset{\sim}{x}_{j+1} - x_j) - \exp(x_j - \tilde{x}_{j-1}) \end{aligned} \qquad [55]$$

whose Lagrangian function is given by

$$\mathcal{L} = \sum_{k=1}^{N} \psi(\tilde{x}_k - x_k) - h \sum_{k=1}^{N} \exp(x_{k+1} - \tilde{x}_k) \qquad [56]$$

with

$$\psi(\xi) = h^{-1}(\exp(\xi) - 1 - \xi) \qquad [57]$$

The variables β_j acquire the following extremely simple expression in the Lagrangian coordinates $x_j, \tilde{x}_j$:

$$\beta_j = \exp(\tilde{x}_j - x_j)$$

For integrable Hamiltonian systems with long-range two-body interaction, such as Calogero–Moser type systems, and their so-called relativistic version (Ruijsenaars systems), an exact integrable discretization has also been found. However, at least

in the more natural Lax representation, the related R-matrix is dynamical (namely, it depends on the phase-space coordinates), and the simple factorization scheme holding for the Toda lattice system (and for the related ones) is not available.

Further knowledge on the intriguing subject of "discrete integrable systems" can be acquired by looking at the monographs and papers listed in the "Further Reading" section. In particular, the excellent book by Y B Suris, which also provides an exhaustive list of references (updated to 2003), is recommended.

See also: Billiards in Bounded Convex Domains; Boundary Value Problems for Integrable Equations; Calogero–Moser–Sutherland Systems of Nonrelativistic and Relativistic Type; Integrable Systems and Discrete Geometry; Integrable Systems and the Inverse Scattering Method; Integrable Systems: Overview; Painlevé Equations; Quantum Calogero–Moser Systems; Toda Lattices; Yang–Baxter Equations.

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Integrable Systems and Algebraic Geometry

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Historical Overview

The relevance of algebraic geometry in the theory of dynamical systems has a long history. Three models may serve as guiding threads from old to the current state of the theory. Each time algebraic geometry is used to integrate an evolution equation; this is achieved by an underlying addition rule. The very origin for this seems to be Fagnano's addition rule for the arc of a lemniscate (see Siegel (1969)). In analogy to the addition of two arcs on a circle $x^2 + y^2 = 1$, or the duplication formula for

$$\arcsin r = \int_0^r \frac{\mathrm{d}r}{\sqrt{1-r^2}}$$

namely

$$\int_0^r \frac{\mathrm{d}r}{\sqrt{1-r^2}} = 2\int_0^u \frac{\mathrm{d}u}{\sqrt{1-u^2}}$$

if $r = 2u\sqrt{1-u^2}$ (a restatement of the trigonometric identity $r = \sin(2x) = 2\sin x \cos x$), Fagnano found, and proved, by substitution, a geometric rule for duplicating the arc of a lemniscate:

$$x^4 + 2x^2y^2 + y^4 = x^2 - y^2$$

The length of the arc is now given by

$$s = \int_0^r \frac{\mathrm{d}r}{\sqrt{1-r^4}}$$

and later Gauss designated the limit of integration by $r = \mathrm{sinlemn}(s)$. Fagnano was able to show that

$$\int_0^r \frac{\mathrm{d}r}{\sqrt{1-r^4}} = 2\int_0^u \frac{\mathrm{d}u}{\sqrt{1-u^4}}$$

with the substitution

$$r^2 = \frac{4u^2(1-u^4)}{(1+u^4)^2}$$

which is remarkable not only because it doubles the length, but also because it does so by rational functions, and in fact shows that the arc of the lemniscate can be halved by straightedge and compass. Gauss showed that the constructible fractions of an arc of a lemniscate are the same as the ones for the circle.

Thanks to subsequent work by Euler, and to the theory of abelian functions due to Abel, Jacobi, and others in the nineteenth century, we now realize that Fagnano's discovery revealed the algebraic group structure of the singular quartic curve (or of a smooth cubic, if preferred, an elliptic curve).

This is the key fact that provides the "integration by quadratures" for the simple pendulum. We follow McKean and Moll (1997) to sketch this prototype example of a system which is algebraically completely integrable (ACI), defined in the section

"Hitchin systems." Newton's law gives the equation of motion $\ddot{\theta} + \sin\theta = 0$, where θ parametrizes the position of the bob in terms of the angle the pendulum makes with the vertical axis, as it rotates about its pivot (the length has been normalized so as to match the gravitational constant). The energy is a first integral, $I = \cos\theta - 1/2\dot{\theta}^2$, and the substitution

$$x = \sqrt{\frac{2}{1-I}} \times \sin\frac{\theta}{2}$$

linearizes the motion:

$$t = \int_0^x \frac{1}{\sqrt{(1-x^2)(1-k^2x^2)}}\,\mathrm{d}x$$

with $k^2 = (1-I)/2$ between 0 and 1, precisely because of Fagnano's and Euler's addition rule.

The second striking example of addition rule, yielding solutions to a nonlinear partial differential equation (PDE), together with this first will provide the two themes of this article, and embed into an infinite-dimensional family of conservation laws that will accommodate the representation-theoretic aspect of the symmetries. In their 1895 article, Korteweg and de Vries (KdV) gave official status to the (then controversial) representation of solitary waves in shallow water:

$$u_t = 6uu_x - u_{xxx}$$

(again up to normalization) is by now the well-known KdV equation, where u represents the amplitude of the wave and x the direction along a canal. It so happens that by integrating twice the ordinary differential equation (ODE) obtained by the one-wave ansatz, $z = x - ct$ (where c is the constant velocity), one sees that the solution u and its derivative $u_z = u'$ satisfy identically an algebraic equation:

$$\begin{gathered} -cu' - 6uu' + u''' = 0 \\ (-cu - 3u^2 + u'' + a)u' = 0 \\ \frac{(u')^2}{2} = u^3 + c\frac{u^2}{2} - au + b \end{gathered}$$

$$\begin{aligned} u &= 2\wp + \text{const.} \quad \text{(up to a linear transformation)} \\ (\wp')^2 &= 4\wp^3 - g_2\wp - g_3 = 4(\wp - e_1)(\wp - e_2)(\wp - e_3) \end{aligned}$$

In disguise, then, the PDE and the Hamiltonian evolutions are the same; the motion becomes linear (and quasiperiodic) on the torus $\mathbb{C}/\Lambda$, where Λ is the period lattice of the $\wp$ function. It took considerably greater effort to generalize this correspondence to higher genus. This article is devoted to such a correspondence as well as some of the surprising connections between complete integrability and other areas of mathematics such as: representation theory (the corresponding geometric objects are Grassmann manifolds as opposed to Jacobians); differential algebras (Weyl algebras, commutative rings of differential operators, and differential Galois theory); and reduction in symplectic geometry.

It is often helpful to highlight the relevant features in the simplest example, even if it is of special kind. The KdV equation and, as Hamiltonian counterpart, Neumann's system (see Neumann (1859)) will serve best. The abelian sum identified by Fagnano cannot be defined on points of a curve X of genus $g > 0$; what one can add are points of the g-fold symmetric product $X^{(g)}$ up to linear equivalence, defining (up to noncanonical isomorphism) an abelian variety, the Jacobian $\mathrm{Jac}(X) = \mathbb{C}^g/\Lambda$; analytically, the Jacobian is described by abelian coordinates $z_1, \ldots, z_g$: if $\alpha_1, \ldots, \alpha_g, \beta_1, \ldots, \beta_g$ is a basis of 1-cycles on X with standard intersection matrix and $\omega_1, \ldots, \omega_g$ is the dual basis of holomorphic differentials, then $z_j = \sum_{i=1}^{g} \int_{P_0}^{P_i} \omega_j$ is defined in terms of a fixed base point $P_0 \in X$ and of $(P_1, \ldots, P_g) \in X^{(g)}$ up to the period lattice Λ. It is in these coordinates that the Hamiltonian flows become linear. In canonical coordinates $q_1, \ldots, q_{g+1}, p_1, \ldots, p_{g+1}$, the harmonic oscillator

$$\begin{aligned} \dot{q}_i &= p_i \\ \dot{p}_i &= -e_i q_i \end{aligned}$$

when constrained to the unit sphere $\sum_{i=1}^{g+1} q_i^2$ has equations

$$\begin{aligned} \dot{q}_i &= p_i \\ \dot{p}_i &= -e_i q_i + q_i \sum_j (e_j q_j^2 - p_j^2) \end{aligned}$$

This system is completely integrable in the sense that there exist enough involutory invariants, g generically (in the (q_i, p_i) variables) independent functions on the $2g$-dimensional tangent bundle of the unit sphere with canonical symplectic structure; in fact the coefficients of the polynomial

$$f(\lambda) = \prod_{i=1}^{g+1} (\lambda - e_i)^2 \left(\left(\sum_{k=1}^{g+1} \frac{q_k^2}{\lambda - e_k} \right) \left(\sum_{k=1}^{g+1} \frac{p_k^2}{\lambda - e_k} + 1 \right) - \left(\sum_{k=1}^{g+1} \frac{q_k p_k}{\lambda - e_k} \right)^2 \right)$$

are invariant and the hyperelliptic Riemann surface X whose model in the affine plane is given by $\mu^2 = f(\lambda)$ is called the spectral curve of the system. Since the polynomial $f(\lambda)$ is monic of degree $2g+1$ and has generically simple roots, X has

genus g. A change of variables permits integration by quadratures,

$$q_i(t) = \frac{\vartheta[\eta_{2i-1}](0)\vartheta[\eta_{2i-1}](z_0 - \Delta + 2\sqrt{-1}tU)}{\vartheta[0](0)\vartheta[0](z_0 - \Delta + 2\sqrt{-1}tU)}$$

where z_0, $U \in \mathbb{C}^g$ are constant vectors, $\boldsymbol{\vartheta}$ denotes the Riemann theta function of X, $\eta_k (k = 1, \ldots, 2g)$ are theta characteristics and Δ is the Riemann constant. While these are technical objects of classical Riemann function theory whose detailed definition is best found in a textbook (see, e.g., Mumford (1984)), the point here is that the motion is linearized along the line with direction U, on the hyperelliptic Jacobian Jac(X), which is a $2^{g+1}:1$ cover of the phase space.

A yet deeper fact links the integrable Hamiltonian motion and the (soliton) PDE, namely the statement that $\sum_{i=1}^{g+1}(e_i q_i^2 + p_i^2) = u(t_1, t_3)$ solves the KdV equation, where the variables are renamed as $x = t_1, t = t_3$ to denote two of the g commuting Hamiltonian flows.

The Neumann system as well allows us to uncover another deep relation between dynamics and geometry, namely the moduli aspect: on the one hand, Mumford (1984) used the Neumann system to recover the equation of the spectral curve from a vanishing property of theta functions with characteristics, thereby giving the first characterization of the moduli subvariety of hyperelliptic curves in terms of thetanulls (for any genus). On the other hand, Françoise (1987) explored the relevance of the integrable system to the Picard–Fuchs equations. The fundamental link is provided by Arnol'd's theory, according to which a set of action-angle variables (q_i, p_i), $i = 1, \ldots, n$, for a completely integrable Hamiltonian system can be calculated in terms of a basis γ_i of the first homology of the fibers, which are n-dimensional tori, $\int_{\gamma_j} \mathrm{d}q_i = \delta_{ij}$; hence, in the case of an algebraically integrable system such as the Neumann example (or, in Françoise's paper, the Kowalevski top), in principle one can express the (coefficients of the) differential equations satisfied by the periods in terms of the commuting Hamiltonians, despite the fact that periods and Hamiltonians are transcendental functions the ones of the others. A more general family of period matrices is subject to the Gauss–Manin connection, and the question of whether its general abelian variety is Lagrangian with respect to a holomorphic symplectic structure on the family yields a cubic condition on the periods (Donagi and Markman 1996).

These are two major applications of PDEs to algebraic geometry: characterizing subvarieties of moduli spaces (of curves) and expressing the Gauss–Manin connection acting on sections of a Hodge-theoretic bundle over the moduli space in terms of the evolution equations of a completely integrable system. In the former case, the flows of the system act on the theta functions of a (fixed) curve; in the latter, the Hamiltonians are related, via the action variables, to computing the monodromy over the branch points of the base of the system. The generalization of specific (e.g., hyperelliptic) cases is very difficult to work out and remains largely open 40 years after the field of integrable equations started being actively investigated.

Before concluding this historical overview, a beautiful theory that escaped attention is worth mentioning. In the late nineteenth century, for example, Baker (1907) constructed the first genus-2 solutions of the KdV equation, although he was apparently not aware of the equation itself; in the process, he also defined what is known as the Hirota bilinear operator, a device introduced by R Hirota in the 1970s to capture an equivalent version of the KdV, or the more general Kadomtsev–Petviashvili (KP) equation,

$$(u_t - 6uu_x + u_{xxx})_x = u_{yy}$$

Just as the Lax pair allows for a linearization of the isospectral deformations, Hirota's bilinear form reveals the representation-theoretic (and algebro-geometric) nature of the equations, via the vanishing of a natural pairing on a pair of solutions, besides providing a formula for exact solutions; the definition of the bilinear operation is the following: for functions F and G,

$$D_{t_n} F \cdot G = \left(\frac{\partial}{\partial t'_n} - \frac{\partial}{\partial t_n} \right) F(\underline{t}) G(\underline{t}') |_{\underline{t}=\underline{t}'}$$
$$\underline{t} = (t_1, t_2, \ldots)$$

so that Hirota's direct method gives the following solution: set $u = 2(\partial^2/\partial x^2) \log F$, then

$$\mathrm{KdV} \Leftrightarrow (D_x D_t + D_x^4) F \cdot F = 0$$

$$\mathrm{KP} \Leftrightarrow D_x^2 \frac{\left(D_x^4 + 3D_y^2 - 4D_x D_t\right) F \cdot F}{2F^2} = 0$$

Baker was intent on generalizing the properties of the Weierstrass $\wp$ function. He focused on genus 2 (and obtained partial results for general genus), in which case any curve is hyperelliptic,

$$f : \mu^2 = \lambda^{2g+1} + a_{2g}\lambda^{2g} + \cdots + a_0$$

and used a suitable basis of holomorphic differentials particular to the hyperelliptic case, whose

integrals give abelian coordinates z_i that happen to be dual to the KdV flows,

$$\omega_1 = \frac{d\lambda}{2\mu},\ \omega_2 = \frac{\lambda d\lambda}{2\mu},\ \ldots,\ \omega_g = \frac{\lambda^{g-1} d\lambda}{2\mu}$$

to characterize the genus-2 theta function by differential equations (equivalent to the KdV hierarchy), as well as give the quartic equation for the Kummer surface in $\mathbb{P}^3$, namely the 2:1 image of the Jacobian of the curve mapped by the divisor 2Θ, that is, by a basis of the space of theta functions with second-order characteristics, simply as the determinant of

$$\begin{bmatrix} -a_0 & \frac{1}{2}a_1 & 2\wp_{11} & -2\wp_{12} \\ \frac{1}{2}a_1 & -(a_2+4\wp_{11}) & \frac{1}{2}a_3+2\wp_{12} & 2\wp_{22} \\ 2\wp_{11} & \frac{1}{2}a_3+2\wp_{12} & -(a_4+4\wp_{22}) & 2 \\ -2\wp_{12} & 2\wp_{22} & 2 & 0 \end{bmatrix}$$

where

$$\wp_{ij}(z) = -\frac{\partial^2}{\partial z_i \partial z_j} \log \sigma(z)$$

and the σ function, defined in analogy to the genus-1 case, is proportional to the Riemann theta function.

To summarize this introduction, the exchange between algebraic geometry (the classification of algebraic varieties) and dynamical systems has been extremely fruitful in either direction: algebraic geometry surprisingly provides exact solutions to evolution equations that have special algebraic symmetries (and arise in nature!), and conversely those very evolutionary equations yield the structure of particularly complicated varieties, by characterizing their (rational) functions.

Isospectral Deformations

The isospectral deformations in question have been encoded by Lax-pair equations, which take their name from Peter D Lax, who gave a version of the KdV equation in such form.

Lax pairs enter in two essentially different ways in the theory of integrable systems. The evolution equations take the form: $\partial_{t_n} L = [B, L]$, where $t_1, t_2, t_3, \ldots$ is a sequence of commuting time flows, L is an operator whose coefficients depend on time, and B is another operator of the same kind; since heuristically this is the infinitesimal version of the equation $L(t) = U(t)^{-1} L(0) U(t)$ (with $B = U^{-1}\partial_t U$), the spectrum of L is preserved and provides conserved quantities; in fact, Moser (1980) speculated that every completely integrable system might have such a form.

In the form that immediately yields a hierarchy of PDEs, the (hierarchy of) deformations pertain to a ring of (formal) pseudodifferential operators, where the variable $x = t_1$ is singled out and ∂ denotes differentiation with respect to x:

$$L(t) \in \mathcal{D} = \left\{ \sum_{j=0}^{n} u_j(x)\partial^j, u_j \text{ analytic near } x = 0 \right\}$$

$$\subset \mathcal{P} = \left\{ \sum_{-\infty}^{n} u_j(x)\partial^j \right\}$$

The multiplication rule that makes $\mathcal{P}$ into a ring (in fact, a $\mathbb{C}$-algebra) is composition:

$$\partial \circ u = u\partial + u'$$
$$\partial^{-1} \circ u = u\partial^{-1} - u'\partial^{-2} + u''\partial^{-3} - \cdots$$

We normalize L by an automorphism of $\mathcal{D}$ (generated by a change of variable and conjugation by a function)

$$L = \partial^n + u_{n-2}(x)\partial^{n-2} + \cdots + u_0(x)$$

In $\mathcal{P}$ any (normalized) L has a unique nth root, $n = \operatorname{ord} L$, of the form $\mathcal{L} = \partial + u_{-1}(x)\partial^{-1} + u_{-2}(x)\partial^{-2} + \cdots$. Finally, the deformation equations,

$$\partial_{t_n} \mathcal{L} = [(\mathcal{L}^n)_+, \mathcal{L}]$$

define the KP hierarchy, which takes its name from the first nontrivial deformation equation, known as the KP equation encountered above, if we set $x = t_1, y = t_2, t = t_3$ (notice that this reduces to KdV, up to rescaling, when the solution is independent of y). The algebro-geometric solutions are those with the property that only a finite number of time evolutions are independent. This turned out to be equivalent to a classical problem of elementary differential algebra, known as the Burchnall–Chaundy problem after the two co-authors who solved it in the 1920s.

The Burchnall–Chaundy problem: which $L(x)$'s have centralizer $\mathcal{C}_\mathcal{D}(L)$ that is larger than a polynomial ring $\mathbb{C}[L_1]$, $L_1 \in \mathcal{D}$? The key to the solution is the following fact (which clearly does not hold for operators in more than one variable, or finite-dimensional operators such as matrices): if $\operatorname{ord} L > 0$ and $A, B \in \mathcal{D}$ both commute with L, then $[A, B] = 0$; in particular, $\mathcal{C}_\mathcal{D}(L)$ is commutative, hence every maximal-commutative subalgebra of $\mathcal{D}$ is a centralizer. It was proved in the early 1900s by I Schur that $\mathcal{C}_\mathcal{D}(L) = \{\sum_{-\infty}^{N} c_j \mathcal{L}^j, c_j \in \mathbb{C}\} \cap \mathcal{D}$. It follows that centralizers are rings of affine curves: their transcendence degree over the field of coefficients is 1, and $\operatorname{Spec} \mathcal{C}(L)$ can be regarded as an affine curve X_0 (with natural compactification

X by a smooth point at infinity). Burchnall and Chaundy proceeded to show that the rings of operators whose orders are not all multiples of a fixed integer >1, and having the same spectral curve X (up to isomorphism), correspond to line bundles over X (more precisely, rank-1 torsion-free sheaves); thus, the hierarchy of evolutions linearizes on Jac X, as indicated by the examples treated above.

In this setting, it has been very challenging to generalize the integrable flows, both to the higher-rank and to the higher-dimensional case. When all the operators in the commutative ring have order divisible by an integer $r > 1$, their common kernel defines a rank-r vector bundle over the spectral curve, and although the theory in principle is similar to the case of line bundles, there are no explicit formulas for solution. On the other hand, in order that the spectrum be a variety X of dimension $d > 1$ rather than a curve, it is natural to seek commutative rings of partial differential operators in d variables; but again, while some constructions work in principle, explicit formulas are elusive.

The form in which Lax pairs occur for finite-dimensional Hamiltonian systems is quite different: here what is preserved is the spectrum of a finite-dimensional linear operator, a matrix. The first examples, from which the theory took off, were inspired guesses. The Neumann system described above fits in the following theory: Moser (1980) showed that the Neumann system together with other important classical examples are special cases of rank-2 perturbations (since $(2 = \dim\langle \boldsymbol{p}, \boldsymbol{q}\rangle)$) which preserve the spectrum of a matrix

$$L = A + a\boldsymbol{q} \otimes \boldsymbol{q} + b\boldsymbol{q} \otimes \boldsymbol{p} + c\boldsymbol{p} \otimes \boldsymbol{q} + d\boldsymbol{p} \otimes \boldsymbol{p}$$

where A is a fixed constant matrix which can be normalized to a diagonal, $\mathrm{diag}(e_1, \ldots, e_{g+1})$,

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} \neq 0$$

and $\boldsymbol{u} \otimes \boldsymbol{v}$ denotes the matrix $[u_i v_j]$. The symplectic structure is the standard $\omega = \sum \mathrm{d}p_i \wedge \mathrm{d}q_i$ so that a Hamiltonian H defines a flow

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

and

$$\frac{\partial G}{\partial t} = -\{H, G\} = \sum \frac{\partial H}{\partial p_i}\frac{\partial G}{\partial q_i} - \frac{\partial G}{\partial p_i}\frac{\partial H}{\partial q_i}$$

The Hamiltonian flow of

$$H = \frac{1}{2}\Bigg(a\langle B\boldsymbol{q}, \boldsymbol{q}\rangle + (b + c)\langle B\boldsymbol{q}, \boldsymbol{p}\rangle + d\langle B\boldsymbol{p}, \boldsymbol{p}\rangle - \frac{ad - bc}{2}\sum_{i \neq j} \frac{b_i - b_j}{e_i - e_j}(q_i p_j - q_j p_i)^2 \Bigg)$$

(where $B = \mathrm{diag}(b_1, \ldots, b_{g+1})$ is any fixed diagonal matrix) is equivalent to the Lax-pair equation $\dot{L} = [M, L]$, where M is a suitable matrix:

$$M = \frac{1}{2}(b - c)[b_i \delta_{ij}] + (ad - bc)\left[\frac{b_i - b_j}{e_i - e_j}(q_i p_j - q_j p_i)\right]$$

The Weinstein–Aronszajn formula

$$\det\left(I_n - \sum_{i=1}^{r} \xi_i \otimes \eta_i \right) = \det\Big(I_r - [\langle \xi_i, \eta_j \rangle] \Big)$$

(where each of the $\xi_1, \ldots, \xi_r, \eta_1, \ldots, \eta_r$ is a $(g + 1 = n)$-vector) gives for the spectral invariants

$$\begin{aligned} \frac{l(\lambda)}{e(\lambda)} &= \frac{\det(\lambda - L)}{\det(\lambda - A)} \\ &= \det(I - ((\lambda - A)^{-1}\boldsymbol{q}) \otimes (a\boldsymbol{q} + b\boldsymbol{p}) \\ &\quad - ((\lambda - A)^{-1}\boldsymbol{p}) \otimes (c\boldsymbol{q} + d\boldsymbol{p})) \\ &= \det(I_2 - W_\lambda(\boldsymbol{q}, \boldsymbol{p})) \end{aligned}$$

with

$$W_\lambda(\boldsymbol{q}, \boldsymbol{p}) = \begin{bmatrix} \langle (\lambda - A)^{-1}\boldsymbol{q}, \boldsymbol{q}\rangle & \langle (\lambda - A)^{-1}\boldsymbol{q}, \boldsymbol{p}\rangle \\ \langle (\lambda - A)^{-1}\boldsymbol{q}, \boldsymbol{p}\rangle & \langle (\lambda - A)^{-1}\boldsymbol{p}, \boldsymbol{p}\rangle \end{bmatrix} \times \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

and $\det(I - W_\lambda(\boldsymbol{q}, \boldsymbol{p})) = 1 - \mathrm{tr}\, W_\lambda + \det W_\lambda = 1 - \phi_\lambda(\boldsymbol{q}, \boldsymbol{p})$, defining the rational function ϕ_λ.

Moser also showed that the system is completely integrable and linearizes on the (generalized) Jacobian of the curve $\mu^2 = e^2(\lambda)\phi_\lambda(x, y)$. Letting $a = -1$, $b = -c = 1, d = 0$ gives the Neumann system.

The dilation $\boldsymbol{q} \mapsto \lambda \boldsymbol{q}$ gives a Lax pair with a parameter, $A \mapsto A + \lambda^2 \boldsymbol{q} \otimes \boldsymbol{q} + \lambda(\boldsymbol{q} \otimes \boldsymbol{p} - \boldsymbol{p} \otimes \boldsymbol{q})$, which makes the spectral curve look more natural. Indeed,

Remark (Adler and van Moerbeke 1980). The Neumann flow is equivalent to the Lax pair: $\dot{L}_1 = [M_1, L_1]$, where $L_1 = A\mu^2 + \mu(\boldsymbol{q} \otimes \boldsymbol{p} - \boldsymbol{p} \otimes \boldsymbol{q}) + \boldsymbol{q} \otimes \boldsymbol{q}$ and $M_1 = A\mu + \boldsymbol{q} \otimes \boldsymbol{p} - \boldsymbol{p} \otimes \boldsymbol{q}$. Moreover, the Hamiltonians are of Adler–Kostant–Symes (AKS) type, namely projections (with respect to an ad-invariant inner product) of gradients of orbit-invariant functions to half of the splitting of a Lie algebra.

Specifically, $\{\sum_{-\infty}^{N} A_j\mu^j | A_j \in \mathrm{gl}(n, \mathrm{C})\} = K \oplus N$, with $K = \{\sum_0^N A_j\mu^j\}$ and $N = \{\sum_{-\infty}^{-1} A_j\mu^j\}$; if the inner product is $\langle A, B\rangle = \sum_{i+j=-1} \mathrm{tr}\, A_iB_j$, the dual of N can be identified with $K = K^{\perp}$, and the Hamiltonian for the Neumann flow can be taken to be $H = \langle (1/2)(L_1\mu^{-2})^2, \mu^3 I_{g+1}\rangle$ under the Lie–Poisson brackets and suitable reduction. The flows linearize on the Jacobian of the (hyperelliptic) curve $\det(L_1 - \eta) = 0$.

It is possible to recover the link between the finite and infinite integrable systems (Neumann and KdV) mentioned in the introductory overview, if we notice that squared eigenfunctions for the Lax operator $L = \mathcal{L}^2 = \partial^2 + u$ become algebraic on the spectral curve: Dubrovin *et al.* (2001) introduced the Baker function, namely the unique function $\psi(x, P)$ with the following properties:

(i) For $|x|$ sufficiently small it is meromorphic on $X \setminus \{P_\infty\}$, with pole divisor bounded by $\delta = P_1 + \cdots + P_g$, independent of x, such that $h^0(\delta - P_\infty) = 0$, and near $P_\infty \psi(x, P)\mathrm{e}^{-xz} = 1 + O(z^{-1})$ is holomorphic, with z chosen to be $\lambda^{1/2}$ in our case.

(ii) We let Ω be the unique meromorphic differential with zeros on δ and a double pole of the form $(-\lambda + \text{holomorphic})\mathrm{d}z^{-1}$ at P_∞. Note: (1) that Riemann–Roch show that Ω is unique. (2) We also get a characterization of the dual Baker function, defined as $\psi(x, \iota P)$ in the hyperelliptic case where ι is the involution $(\lambda, \mu) \mapsto (\lambda, -\mu)$, as meromorphic on $X \setminus \{P_\infty\}$ with poles bounded by δ' and behavior $\mathrm{e}^{-xz}(1 + O(z^{-1}))$ near P_∞, where $\delta + \delta'$ are the $2g$ zeros of Ω. (3) Furthermore, $\Omega = \mathrm{d}\lambda / \mathcal{W}(\psi, \phi)$, where $\mathcal{W}$ is the Wronskian (with respect to the variable x). Then, upon fixing a meromorphic function h, normalized at $P_\infty, h = \lambda^{-1/2} + \text{entire}$, with $g+1$ fixed poles distinct from δ, we have:

If $\rho_j = \mathrm{Res}_{e_j} h\Omega$, $q_j = \sqrt{\rho_j}\psi(x, e_j)$, $p_j = \sqrt{\rho_j}\phi(x, e_j)$, *then* $\Sigma_{j=1}^{g+1} q_j^2 = 1$, $\Sigma_{j=1}^{g+1} q_jp_j = 0$, $\Sigma_{j=1}^{g+1}(e_jq_j^2 + p_j^2) = u(x)$ *and* $\{q_j, p_j\}$ *satisfy the Neumann system.*

Indeed, the constraints follow from the "residue theorem" applied to the differential $h\Omega\psi\phi$ (it has a residue of -1 at P_∞); the differential equations $\ddot{q}_j = e_jq_j - uq_j$ follow from the assumption $L\psi = \lambda\psi$.

The function $u = -2\sum_{k=1}^{g+1}(\sum_{l\neq k} e_l)q_k^2$, evolving under suitable abelian flows, is a solution of the KdV equation; the "times" of the KdV hierarchy are linear combinations of the Neumann Hamiltonians; more precisely, of the invariant vector fields determined by the tangent directions to the image of X in Jac$X$, with Abel map normalized at P_∞, at some point P: $D_P = \sum_{k=1}^{g} \lambda(P)^{g-k} D_k$.

The other way around (Moser–Trubowitz, McKean–van Moerbeke),

If $L = \partial^2 + u(x)$ *is a finite-gap operator and* $e_1, \ldots, e_{g+1}$ *are among the* $2g+1$ *edges of the gaps, there exist constants* $\rho_1, \ldots, \rho_{g+1}$ *so that the functions* $p_j(x) = \sqrt{\rho_j}\psi(x, e_j)$ *satisfy* $\sum_1^{g+1} p_j^2(x) \equiv 1$. *Since* $L\psi_j = e_j\psi_j$, *the* $p_j(x)$ *solve the Neumann system.*

The squared eigenfunctions also provide a natural interpretation for Moser's Lax pair. If V_λ is the kernel of $L - \lambda$, then the Baker function $\psi(x, P)$ and its dual $\phi(x, P)$ give a basis of V_λ except at the branch points $(e_i, 0)$ where $\psi = \phi$. But then the normalized basis of V_λ is related to ψ, ϕ by a constant matrix:

$$\begin{bmatrix} y_0 \\ y_1 \end{bmatrix} = C\begin{bmatrix} \psi \\ \phi \end{bmatrix}$$

while

$$B\begin{bmatrix} \psi \\ \phi \end{bmatrix} = \begin{bmatrix} \mu & 0 \\ 0 & -\mu \end{bmatrix}\begin{bmatrix} \psi \\ \phi \end{bmatrix}$$

if B is the differential operator of the Burchnall–Chaundy ring corresponding to multiplication by μ, so that

$$\begin{bmatrix} -V & U \\ W & V \end{bmatrix}^{\mathrm{T}} = M_B = C\begin{bmatrix} \mu & 0 \\ 0 & -\mu \end{bmatrix}C^{-1}$$

By evaluating at $x = 0$, we find:

$$C = \frac{1}{\mathcal{W}}\begin{bmatrix} \phi' & -\psi' \\ -\phi & \psi \end{bmatrix}\Bigg|_{x=0}$$

with $\mathcal{W} = \psi\phi' - \psi'\phi$. Finally, we calculate:

$$C\begin{bmatrix} \mu & 0 \\ 0 & -\mu \end{bmatrix}C^{-1} = \frac{\mu}{\mathcal{W}}\begin{bmatrix} \psi\phi' + \psi'\phi & 2\psi'\phi' \\ -2\psi\phi & -(\psi\phi' + \psi'\phi) \end{bmatrix}$$

so that $U(\lambda) = \psi\phi' + \psi'\phi$, $V(\lambda) = -2\psi\phi$, $W(\lambda) = 2\psi'\phi'$ are polynomials like the entries of $W_\lambda(q, p) \cdot e^2(\lambda)$, and the fact that $UW + V^2$ does not depend on x expresses the fact that $\mathcal{W} = \text{constant}$.

An object that links the two distinct occurrences of Lax pairs is Sato's infinite-dimensional Grassmann manifold. One particular model will serve as illustration, with more general settings covered by Dickey (2003). Sato defined a one-to-one correspondence between cyclic $\mathcal{D}$-submodules $\mathcal{I}$ of $\mathcal{P}$, namely of the type $\mathcal{I} = \mathcal{D}S$ (which turns out to be equivalent to the property: $\mathcal{P} = \mathcal{I} \oplus \mathcal{P}^{(-1)}$), and subspaces of a ring of formal power series, which make up an infinite-dimensional Grassmann manifold, more

precisely elements of $\mathrm{Gr}^{\emptyset}$, the "big cell." This way, KP can be viewed as deformation of $\mathcal{D}$ modules.

There are two ways to set up the Grassmannian: (1) more direct as a limit of finite-dimensional Grassmannians; (2) more intrinsic, using the rings $\mathcal{D} \subset \mathcal{P}$.

1. Let $\dim V = m + n = N, \mathrm{Gr}(m, V) = \{m - \text{frames } in\ V\}/\mathrm{GL}(m) \hookrightarrow \mathbb{P}(\wedge^m V)$ via $\xi^{(0)}, \dots, \xi^{(m-1)} \mapsto \xi^{(0)} \wedge \cdots \wedge \xi^{(m-1)}$.

If we fix a basis $e_0, \dots, e_{N-1}$ of V, and write a frame in coordinates, $\xi^{(i)} = \xi_{0,i} e_0 + \cdots + \xi_{N-1,i} e_{N-1}$, then

$$\xi^{(0)} \wedge \cdots \wedge \xi^{(m-1)} = \sum_{0 \le \ell_0 < \cdots < \ell_{m-1} < N} \xi_{\ell_0 \dots \ell_{m-1}} e_{\ell_0} \wedge \cdots \wedge e_{\ell_{m-1}}$$

with $\xi_{\ell_0 \dots \ell_{m-1}} = \det(\xi_{\ell_i, j})_{i,j=0,\dots,m-1}$

A point in the ambient $\mathbb{P}(\wedge^m V)$ lies in the embedded $\mathrm{Gr}(m, V) \Leftrightarrow$ its projective coordinates $\xi_{\ell_0 \dots \ell_{m-1}} (0 \le \ell_i < N)$ satisfy the Plücker relations (PRs):

$$\sum_{i=0}^{m} (-1)^i \xi_{k_0 \dots k_{m-2} \ell_i} \xi_{\ell_0 \dots \hat{\ell}_i \dots \ell_m} = 0$$

Therefore,

$$\mathrm{Gr}(m, V) = (\widetilde{\mathrm{Gr}}(m, V) \backslash \{0\}) / \mathrm{GL}(1)$$

where $\widetilde{\mathrm{Gr}}(m, V) = \{(\xi_Y)_{Y \subset \Delta_{mN}}$ satisfying the PRs$\}$ is a line bundle over $\mathrm{Gr}(m, V)$, Y is a Young diagram consisting of rows

$$\boxed{\ell_{m-1} - (m-1)}$$
$$\vdots$$
$$\boxed{\ell_1 - 1}$$
$$\boxed{\ell_0}$$

so it is contained in the rectangle Δ_{mN}.

For the commutative diagram:

$$\begin{array}{ccc} \widetilde{\mathrm{Gr}}(m', N') & \overset{\text{project}}{\longrightarrow} & \widetilde{\mathrm{Gr}}(m, N) \\ \downarrow \text{identity} & & \downarrow \text{identity} \\ \widetilde{\mathrm{Gr}}(m', N') & \overset{\text{embed}}{\hookleftarrow} & \widetilde{\mathrm{Gr}}(m, N) \end{array}$$

the following facts can be checked. Let $m \le m', n \le n', N' = m' + n'$:

(i) if $(\xi'_Y)_{Y \subset \Delta_{m'N'}}$ satisfies PRs, so does its restriction to Y's within Δ_{mN};
(ii) if $(\xi_Y)_{Y \subset \Delta_{mN}}$ satisfies PRs, so does $(\xi'_Y)_{Y \subset \Delta_{m'N'}}$ where $\xi'_Y = 0$ unless $Y \subset \Delta_{mN}$.

These facts make it possible to define: $\mathrm{Gr} = (\widetilde{\mathrm{Gr}} \backslash \{0\}) / \mathrm{GL}(1)$, where $\widetilde{\mathrm{Gr}} = \{(\xi_Y)_{Y \text{ all Young diagrams}}$ satisfying all PRs$\}$

$$\begin{array}{ccc} \widetilde{\mathrm{Gr}} & \overset{\text{project}}{\longrightarrow} & \widetilde{\mathrm{Gr}}(m, N) \\ \uparrow \text{dense} & & \downarrow \text{identity} \\ \widetilde{\mathrm{Gr}}^{\text{fin}} & \overset{\text{embed}}{\hookleftarrow} & \widetilde{\mathrm{Gr}}(m, N) \end{array}$$

and

$$\begin{aligned} \widetilde{\mathrm{Gr}}^{\text{fin}} &= \{(\xi) \in \widetilde{\mathrm{Gr}} : \xi_Y = 0 \text{ for almost all } Y\} \\ &= \bigcup_{m,N} \widetilde{\mathrm{Gr}}(m, N) \end{aligned}$$

The KP time deformations are defined as follows:

$$\xi_Y(t) := \sum_{\text{all } Y'} \chi_{Y'/Y}(t) \xi_{Y'} \text{ where } \chi_{Y'/Y}(t) := \det(p_{\ell'_i - \ell_j}(t))$$
$$p_0(t) = 1, p_n(t) := \sum_{\nu_1 + 2\nu_2 + 3\nu_3 + \cdots = n} t_1^{\nu_1} t_2^{\nu_2} \dots / (\nu_1! \nu_2! \dots)$$

Write $\chi_{Y/\emptyset}$ as χ_Y, where $\chi_Y(t) = \det(p_{\ell_i - j}(t))$ are the Schur functions.

To connect with the KP hierarchy, let

$$w_n(x, t) := (-1)^n \frac{\xi_{\Delta_{n,1}}(x + t)}{\xi_\emptyset(x + t)}$$

where $x + t = (x + t_1, t_2, \dots)$, and $S := 1 + w_1(x, t) \partial^{-1} + \cdots$. Then $\mathcal{L} = S \partial S^{-1}$ satisfies the KP hierarchy, namely $\partial_{t_n} S = B_n S - S \partial^n$, where $B_n := (S \partial^n S^{-1})_+, \Longleftrightarrow [\partial_{t_n} - B_n, \partial_{t_k} - B_k] = 0 \Longleftrightarrow \partial_{t_n} \mathcal{L} = [(\mathcal{L}^n)_+, \mathcal{L}]$.

Note The Plücker coordinate $\xi_\emptyset(t) = \sum_{\text{all} Y} \chi_Y(t) \xi_Y = \tau(\xi, t)$ is a generating function for the Plücker coordinates, $\xi_Y(t) = \chi_Y(\partial_t) \xi_\emptyset(t)$, where

$$\partial_t := \left(\frac{\partial}{\partial t_1}, \frac{1}{2} \frac{\partial}{\partial t_2}, \frac{1}{3} \frac{\partial}{\partial t_3}, \dots \right)$$

Now by reducing to $\mathrm{Gr}(m, N)$ and checking that every $\xi_Y(t)$ satisfies PRs, we have a dynamical system on $\widetilde{\mathrm{Gr}}$.

Conclusion (Sato). Although any $f(t) \in \mathbb{C}[[t_1, t_2, \dots]]$ admits a formal expression of the form $\sum_Y c_Y \chi_Y(t)$, where the coefficients are

$$c_Y = \chi_Y(\partial_t) f(t)|_{t=0}$$

it represents the τ function for some $\xi \in \widetilde{\mathrm{Gr}} \Longleftrightarrow$ its coefficients satisfy the following PRs:

$$\sum_{i=0}^{m} (-1)^i \chi_{k_0 \dots k_{m-1} \ell_i} \left(\frac{\partial_t}{2} \right) \chi_{\ell_0 \dots \hat{\ell}_i \dots \ell_m} \left(-\frac{\partial_t}{2} \right) \tau \cdot \tau = 0$$

which is the KP hierarchy in Hirota bilinear form.

2. Let

$$V := \frac{\mathcal{P}}{\mathcal{P}x} \cong \mathcal{P}_{\text{const}} = \left\{ \sum_{-\infty<i<<\infty} a_i \partial^i,\ a_i \in \mathbb{C} \right\}$$

equipped with the induced filtration $V^{(i)}$ by order, induced by

$$\mathcal{P}^{(i)} = \left\{ \sum_{-\infty<k\leq i} a_k \partial^k,\ a_k \in \mathbb{C} \right\}$$

and define

$$\begin{aligned} \text{Gr} = \{&\text{vector subspaces } W \text{ of } V \\ &\text{s.t.} \dim(W \cap V^{(0)}) = \dim V/(W + V^{(0)}) < \infty\} \end{aligned}$$

"same size" as the reference subspace $\{\sum_{\nu\leq 0} c_\nu e_\nu : c_\nu \in \mathbb{C}\} = V^{(0)}$.

The correspondence between such a W and a cyclic submodule of $\mathcal{P}$ is given as follows:

$$\begin{aligned} \mathcal{I} &\mapsto W = S^{-1}V^{(0)} = \{v \in V : \mathcal{I}v \subset V^{(0)}\} \\ W &\mapsto \mathcal{I} = \{A \in \mathcal{P} : AW \subset V^{(0)}\} \end{aligned}$$

Generic points of particular interest in constructing KP solutions make up the "big cell":

$$\begin{aligned} \text{Gr}^{\emptyset} \underset{\text{open dense}}{\subset} \text{Gr} &\Longleftrightarrow V = W \oplus V^{(0)} \\ &\Longleftrightarrow \xi_\emptyset \neq 0 \text{ and a } \tau \text{ function can} \\ &\qquad \text{be defined as above} \end{aligned}$$

In standard basis of $V, e_i := \partial^{-i-1} \bmod \mathcal{P}x,\ i \in \mathbb{Z}$, the action

$$\begin{aligned} xe_i &= (i+1)e_{i+1} \\ \partial e_i &= e_{i-1} \end{aligned}$$

gives V a $\mathcal{P}$-module structure. Let Λ be the shift operator: $\partial e_i = e_{i-1}$; then

$$\xi(t) = \mathrm{e}^{(t_1\Lambda + t_2\Lambda^2 + \cdots)} \cdot \xi$$

so, this linearizes the flows!

This survey would not be complete without an example of the formula that links the τ and the theta function; more general statements and groups of symmetries can be found in Dickey (2003). A solution of the KP hierarchy can be expressed in terms of the τ function τ_W associated with an element W of Gr(H), in the model Gr(H), where $H = L^2(S^1), H = H_+ \oplus H_-$ with standard basis $H_+ = \langle 1, z, z^2, \ldots \rangle, H_- = \langle z^{-1}, z^{-2}, \ldots \rangle$ and $p_\pm$ the projections, $\tau_W(g) = \det(\mu_g \circ p_+ \circ \mu_{g^{-1}} \circ (p_+|_W)^{-1})$, where $g = \mathrm{e}^{\Sigma t_i z^i}$. The associated Baker function $\psi_W(g, z)$ is a function of the form

$$\psi_W(g, z) = g(z)\left(1 + \sum_{i=-\infty}^{-1} a_i z^i\right)$$

with $a_i \in \mathbb{C}[[t_1, t_2, \ldots]]$ for each i, such that the map $z \mapsto \psi_W(g, z)$ is an element of $g^{-1}W$. If $\phi = 1 + \sum_{i=-\infty}^{-1} a_i z^i$, then $L = \phi\partial\phi^{-1}$ is a solution of the KP hierarchy.

Moreover,

$$g^{-1}\psi_W(g, \zeta) = \frac{\tau_W\left(\left(t_\alpha - \frac{1}{\alpha\zeta^\alpha}\right)\right)_\alpha}{\tau_W((t_\alpha))_\alpha}$$

This is the analog of the expression for the Baker function in terms of the theta function, when W corresponds to an element of the Jacobian of the spectral curve Γ via the Krichever map

$$\begin{aligned} \psi(x, P) &= \exp\left(x \int \eta - xa\right) \\ &\quad \times \frac{\vartheta(Ux + A(P) - A(D) - \Delta)\vartheta(A(D) + \Delta)}{\vartheta(A(P) - A(D) - \Delta)\vartheta(Ux - A(D) - \Delta)} \end{aligned}$$

where $P \in \Gamma, A(-)$ is the Abel map, Δ the Riemann constant, $U \in \mathbf{C}^g$ a suitable vector, D a generic divisor of points $P_1, \ldots, P_g \in \Gamma, \eta$ a differential of the second kind, and a a constant depending on the curve. For the KdV solutions, the condition on $W \in \text{Gr}^{\emptyset}$ is that $z^2 W \subset W$ and the solution is

$$u_W(x, t_2, t_3, \ldots) = 2\partial \log \tau_W(x, t_2, t_3, \ldots)$$

In the Grassmannian formulation, the Hirota bilinear operator mentioned in the introductory overview makes its third and most general appearance (we regard Baker's and Hirota's definitions as the first two – the one based on a residue formula in algebraic geometry, the other on the vanishing of a differential form):

Definitions

(i) In $\mathcal{P}$, it is possible to conjugate any $\mathcal{L} = \partial + u_{-1}(x)\partial^{-1} + \cdots$ into ∂ by a $K = 1 + v_{-1}(x)\partial^{-1} + \cdots$, determined up to elements of $\mathbf{C}[\partial] = \mathcal{C}_{\mathcal{D}}(\partial)$: $K^{-1}\mathcal{L}K = \partial$.

(ii) We define a formal Baker function for $\mathcal{L}$ as the element of the module M (the free, rank-1 $\mathcal{P}$-module = space of formal expressions $f = \mathrm{e}^{xz}\tilde{f}$ where $\tilde{f} = \sum_{-\infty}^{N} f_j(x)z^j$, with generator e^{xz}) such that $\mathcal{L}\psi = z\psi$; so that $\psi = K\mathrm{e}^{xz}$ for K as in (i).

(iii) We say that the formal adjoint $A^\dagger$ of a (formal pseudo) differential operator $A = \sum_{j=-\infty}^{N} u_j(x)\partial^j$ is $A^\dagger = \sum_{j=-\infty}^{N} (-\partial)^j u_j(x)$, and that the dual Baker function $\psi^\dagger$ to $\psi = K\mathrm{e}^{\Sigma t_i z^i}$ is the Baker function of $(\mathcal{L}^\dagger)$; the operator which corresponds to K in (i) is $(K^\dagger)^{-1}$, that is, $(K^\dagger)^{-1}\mathcal{L}^\dagger K^\dagger = -\partial$.

Then, the KP hierarchy is equivalent to the following formula:

$$\text{Res}_z \psi(t', z)\psi^\dagger(t, z) = 0$$

Moreover, as proved in Dickey (2003), if ψ_1 and ψ_2 are formal power series of the form $\psi_1 = Ke^{\Sigma t_i z^i}, \psi_2 = Je^{-\Sigma t_i z^i}$, for $K, J \in 1 + \mathcal{P}^{(-1)}$, satisfying the condition

$$\mathrm{Res}_z\left(\partial_{i_1}^{\alpha_1}\partial_{i_2}^{\alpha_2}\cdots\partial_{i_m}^{\alpha_m}\psi\right)\cdot\phi = 0$$

then there exists an operator $\mathcal{L}$ satisfying the Lax equations, whose wave function and adjoint wave function are ψ_1, ψ_2, respectively.

To conclude this overview of Lax equations, we point out that they can be viewed as zero-curvature condition for a (formal) connection (on the trivial bundle over the formal deformation space whose fiber is $\mathcal{P}$), rephrasing the fact that the time flows commute and hence define time deformations; such formulation can be found in Mulase (1984).

Symplectic Reduction and *r* Matrices

While the Lax-pair presentation provides natural spectral invariants, the group/representation-theoretic nature of integrability (sometimes referred to as hidden symmetries) is best seen in the context of Marsden–Weinstein reduction. We perform it in the example of a generalization of Moser's rank-2 perturbation; we extract the basic construction from Adams *et al.* (1988). A more comprehensive treatment can be found in Babelon *et al.* (2003).

Definition We let $M_{n,r}$ denote the space of $n \times r$ complex matrices, with $n \geq r$ and give $M = M_{n,r} \times M_{n,r}$ the symplectic structure $\omega(F, G) = \mathrm{tr}(\mathrm{d}F \wedge \mathrm{d}G^{\mathrm{T}})$ for $F, G \in M$. A rank-r perturbation of a fixed $n \times n$ matrix A is $L = A + FG^{\mathrm{T}}$.

Definition We split the formal loop algebra $\widetilde{\mathrm{gl}(r)} = \widetilde{\mathrm{gl}(r)}^{+} \oplus \widetilde{\mathrm{gl}(r)}^{-}$ where $\widetilde{\mathrm{gl}(r)}^{+}$ consists of $r \times r$ matricial polynomials in λ and $\widetilde{\mathrm{gl}(r)}^{-}$ of strictly negative formal power series. Under the pairing $\langle X(\lambda), Y(\lambda)\rangle = \mathrm{tr}(X(\lambda)Y(\lambda))_{-}$ (where the subscript $-$ means the coefficient of λ^{-1}), the dual of $\widetilde{\mathrm{gl}(r)}^{+}$ is identified with $\widetilde{\mathrm{gl}(r)}^{-}$, which therefore admits a Lie–Poisson structure.

In sketch, we consider an action on M whose moment map lands in $\widetilde{\mathrm{gl}(r)}^{-}$; we check that the AKS flows on $\widetilde{\mathrm{gl}(r)}^{-}$ correspond to isospectral deformations of $L = A + FG^{\mathrm{T}}$ for flows on M_A; finally, we perform a Marsden–Weinstein reduction for an (equivariant) GL(r) action to obtain a completely integrable system on a symplectic leaf, whose flows are linear on the Jacobian of the spectral curve. We recall very briefly the general definitions.

Moment Map

1. A smooth group action of G on a symplectic manifold (M, ω) is said to be Hamiltonian if there exists a "moment map" $J : M \to g^*$ such that the Hamiltonian vector field associated with J and a fixed element $\xi \in g$ is the same as the infinitesimal action associated with ξ. However, an infinitesimal definition is given because in the formal setup the group of a Lie algebra is often delicate to define. We recall that:
2. The Lie–Poisson structure of g^* is defined by

   $$\{\phi, \psi\}_{g^*}(\mu) = < \mu, [\mathrm{d}\phi(\mu), \mathrm{d}\psi(\mu)] > \quad \text{for } \phi, \psi \in \mathcal{C}^{\infty}(g^*), \quad \mu \in g^*$$

   where $\mathrm{d}\phi : g^* \to g^{**}$ (which in our situation will always be identified with g) is defined by

   $$< \mathrm{d}\phi(\mu), \nu > = \frac{\mathrm{d}}{\mathrm{d}t}\phi(\mu + t\nu)\Big|_{t=0}, \quad \mu, \nu \in g^*$$

   Now we say that $J : M \to g^*$ is a moment map if
3. its linear dual $j : g \to \mathcal{C}^{\infty}(M)$ is a Lie-algebra homomorphism; or if
4. it is a Poisson map with respect to the Lie–Poisson structure: $\phi, \psi \in \mathcal{C}^{\infty}(g^*) \Rightarrow \{J^*\phi, J^*\psi\} = J^*\{\phi, \psi\}_{g^*}$. In case we do have a Hamiltonian G-action, then the subspace $\mathcal{C}^{\infty}_G(M)$ of G-invariant functions is a Lie subalgebra of $\mathcal{C}^{\infty}(M)$. If G acts freely and properly on M, then M/G is a manifold with a Poisson structure inherited from the one on M through the identification $\mathcal{C}^{\infty}(M/G) \cong \mathcal{C}^{\infty}_G(M)$. The symplectic leaves of M/G have the form $M_{\mu} = J^{-1}(\mu)/G_{\mu} = J^{-1}(\mathcal{O}_{\mu})/G$, where $\mu \in g^*$, G_{μ} is the isotropy group of μ in G and $\mathcal{O}_{\mu}$ is the G-orbit through μ. The reduced manifold M_{μ} has a natural symplectic structure ω_{μ} such that $i^*\omega = \pi^*\omega_{\mu}$, where $i : J^{-1}(\mu) \to M$ is inclusion and $\pi : J^{-1}(\mu) \to M_{\mu}$ is the natural projection taking points to their G_{μ}-orbits.

This class of examples can be treated with the technique of a (classical) r-matrix, as follows. Given a linear map $R : g \to g$, the alternating bilinear form $[X, Y]_R = (1/2)([RX, Y] + [X, RY])$ satisfies the Jacobi identity $\Leftrightarrow$ certain quadratic conditions on R are satisfied. Assuming they are, for all pairs of invariant functions I, J on g^*, we have $\{I, J\}_R = 0$ (where $\{\,,\,\}_R$ is the attendant (Lie–Poisson) structure). Indeed, $\{I, J\}_R(\mu) = \langle[\mathrm{d}I(\mu), \mathrm{d}J(\mu)]_R, \mu\rangle = (1/2)\langle[R\mathrm{d}I(\mu), \mathrm{d}J(\mu)], \mu\rangle + (1/2)\langle[\mathrm{d}I(\mu), R\mathrm{d}J(\mu)], \mu\rangle$, but, for example, $\langle[R\mathrm{d}I(\mu), \mathrm{d}J(\mu)], \mu\rangle = \langle R\mathrm{d}I(\mu), \mathrm{ad}^*\mathrm{d}J(\mu)(\mu)\rangle = 0$.

Remark As is clear from the proof above, our definition of invariant need only be infinitesimal, that is, $f \in I(g^*)$ iff $< \mu, [\mathrm{d}f(\mu), X] > = 0 \ \forall \mu \in g^*$, $X \in g$. Of course, when we have a corresponding Lie group the invariants are the functions which are

invariant under the natural action, such as the symmetric functions of the eigenvalues of a matrix.

AKS Flows

For a splitting $g = K \oplus N$, as given above, with $g^* = N^* \oplus K^*$, an example of r-matrix is given by $R(X) = X_+ - X_-$ (where $+,-$ denote projection to K, N): the Jacobi identity is straightforward to check. As a consequence, invariants on g^* are in involution with respect to $\{,\}_R$ and these are called AKS flows, after work done independently by AKS: $\dot{X} = [\mathrm{d}f(\tilde{X})_+, X] = -[\mathrm{d}f(\tilde{X})_-, X]$, given here for the special case in which we can identify K with K^* and $\tilde{X}$ is the element in K^* that corresponds to $X \in K$.

We now proceed to the appropriate moment maps. We generalize the constant matrix A introduced above (isospectral deformations) by allowing multiple eigenvalues α_i of multiplicities $n_i \leq r, n_1 + \cdots + n_k = n$, so that $\det(A - \lambda I) = \prod_{i=1}^k (\alpha_i - \lambda)^{n_i}$. Let $a(\lambda) = \prod_{i=1}^k (\alpha_i - \lambda)$. We split an $n \times r$ matrix F into k blocks F_i accordingly.

Definition/statement

(i) $J_r^n(F, G)(x_1, \ldots, x_n) = -\sum_{j=1}^n \mathrm{tr}(F_j X_j G_j^{\mathrm{T}})$ is the moment map of the action $[(g_1, \ldots, g_n)(F, G)]_i = (F_i g_i^{-1}, G_i g_i^{\mathrm{T}})$, where $g_i \in \mathrm{GL}(r)$ so that under standard identifications $J_r^n(F, G) = -(G_1^{\mathrm{T}} F_1, \ldots, G_n^{\mathrm{T}} F_n)$ and restricting the action to the diagonal subgroup $\{(g, \ldots, g)\}$, $J_r(F, G) = -G^{\mathrm{T}} F$.

(ii) For $X(\lambda) \in \widetilde{\mathrm{gl}(r)}^+$ we define $\alpha(X(\lambda)) = (X(\alpha_1), \ldots, X(\alpha_r))$ and obtain the exact sequence

$$0 \to a(\lambda)\widetilde{\mathrm{gl}(r)}^+ \xrightarrow{\iota} \widetilde{\mathrm{gl}(r)}^+ \xrightarrow{\alpha} g_r^n \to 0$$

By dualizing, and identifying g_r^n to its dual by using the trace componentwise, we get

$$\alpha^*(Y_1, \ldots, Y_n) = \sum_{i=1}^k \frac{Y_i}{\lambda - \alpha_i}$$

and finally check that $\tilde{J}_r = \alpha^* \circ J_r^n$ is a moment map. By combining (i) and (ii), we get a moment map

$$\tilde{J}_r(F, G) = \sum_{i=1}^k \frac{G_i^{\mathrm{T}} F_i}{\alpha_i - \lambda} = G^{\mathrm{T}}(A - \lambda)^{-1} F$$

which becomes injective on $\mathcal{M}/H$, where $\mathcal{M}$ is a suitable open submanifold of M and $H = \mathrm{GL}(n_1) \times \cdots \times \mathrm{GL}(n_k)$ acts blockwise by $(h_i F_i, h_i^{-1\mathrm{T}} G_i)$.

(iii) We also notice that the "Moser space" $M_A = \{A + FG^{\mathrm{T}} | F, G \in \mathcal{M}\}$ of rank-r perturbations can be identified with the orbit space $\mathcal{M}/G_r, G_r = \mathrm{GL}(r)$ acting as in (i).

To finish, we turn on the obvious AKS flows on $\widetilde{\mathrm{gl}(r)}^-$: the key observation is that they are isospectral for the rank-r perturbation $A + FG^{\mathrm{T}}$: we see that the Poisson-commutative ring $\mathcal{F}_+$ of projected invariants defines, by composition with $\tilde{J}_r$, a Poisson-commutative ring $\mathcal{F}$ of isospectral flows on $M_{n,r} \times M_{n,r}$.

Hitchin Systems

The Hitchin system, introduced in the late 1980s, 20 years later still encompasses the most general class of "algebraically completely integrable" systems, which we now discuss. In its most basic form, the concept of "algebraic completely integrable" (ACI) Hamiltonian system, is an extra condition on the integrability of classical mechanics, in the following sense.

A Hamiltonian system with n degrees of freedom, that is, defined on a symplectic manifold M of (real) dimension $2n$ is (Arnol'd–Liouville) completely integrable if it admits n functions in involution whose differentials are linearly independent (possibly, generically on M). When M is a component of the set of real points of an algebraic variety $M_{\mathbb{C}}$ and the symplectic form ω and Hamiltonian function H are rational without poles on M, the concept of algebraic complete integrability can be introduced. For this condition to hold, we require that the vector fields corresponding to the Hamiltonians in involution still have no poles on a compactification of the fibers on $M_{\mathbb{C}}$.

Nonexample (Mumford 1984, §4). Consider

$$M = \mathbb{R}^2, \quad \omega = \mathrm{d}x \wedge \mathrm{d}y, \quad H = x^4 + y^4$$

Here a compactification of the fiber, the affine curve $x^4 + y^4 = c$, is the projective curve $X^4 + Y^4 = cZ^4$, which is smooth (provided $c \neq 0$) and has four points at infinity. The vector field X_H defined by H, $X_H \rfloor \omega = -\mathrm{d}H$, is tangent to the fiber in the affine plane, but has a pole at infinity as can be checked by a change of coordinates; 4 is the lowest exponent for which this simple nonexample works!

Note In the algebraically completely integrable situation, the fibers are abelian varieties or extensions of such by $\mathbb{C}^{*k}$ for some power k. This gives rise to the issues of variations of periods over the base mentioned in the introductory overview.

The Neumann system is ACI, with integral tori given by the Jacobians of the spectral curves:

$$\Gamma : \mu^2 = g(\lambda) = \prod_1^{2g+1} (\lambda - e_i) = UW + V^2$$

where

$$L = e(\lambda)\begin{bmatrix} \sum \frac{q_i p_i}{\lambda - e_i} & \sum \frac{p_i^2}{\lambda - e_i} \\ 1 + \sum \frac{q_i^2}{\lambda - e_i} & -\sum \frac{q_i p_i}{\lambda - e_i} \end{bmatrix} = \begin{bmatrix} V & U \\ W & -V \end{bmatrix}, \quad e(\lambda) = \prod_1^{g+1}(\lambda - e_i)$$

$U = \prod_{i=1}^{g}(\lambda - \lambda_i)$, $(\lambda_1, \ldots, \lambda_g)$ "elliptical spherical coordinates"

$$\psi = \left(1, \frac{U}{V+\mu}\right) \text{ eigenvector: } L\psi = \mu\psi$$

$$\text{divisor: } \sum_{i=1}^{g}(\lambda_i, V(\lambda_i))$$

Hitchin (1982) devised a geometrical model of the spectral curve, a compact algebraic curve contained in the surface $\mathcal{T}^*\mathbb{P}^1$, and its line bundles. He also provided subsequently (1987) a dramatic generalization.

Hitchin's construction, in the Neumann-system example, highlights the following objects:

- $L \in H^0(\mathbb{P}^1, \mathrm{End}(E) \otimes \mathcal{O}(g+1))$, E rank $(r=)2$ bundle over $\mathbb{P}^1$;
- T = total space of the line bundle $\mathcal{O}(g+1)$ over $\mathbb{P}^1$;
- μ = tautological section: $\mathbb{P}^1 \to T$, where $\tilde{L} - \tilde{\mu}I \in H^0(T, \mathrm{End}(\tilde{E}) \otimes \tilde{\mathcal{O}}(g+1))$ (tildes denote pullback);
- Γ: $\det(\tilde{L} - \tilde{\mu}I) = 0$. The line bundle ψ (eigenvectors) is defined as the kernel of $\tilde{L} - \tilde{\mu}I$; and
- the moduli space of spectral curves is a linear system on the surface T. Fixing $\{e_1, \ldots, e_{g+1}\}$ in the above example gives constraints that define it as subsystem of a complete linear system, as well as providing a Poisson structure on the whole $((2g-1)+g)$-dimensional manifold (base = curves, fiber = Jacobians) which reduces to the standard $\sum dp_i \wedge dq_i$. Equivalent to choosing a section $s \in H^0(\mathbb{P}^1, \mathcal{O}(g-1) \otimes K^{-1}_{\mathbb{P}^1})$,

$$\begin{array}{ll} \Gamma & s \leftrightarrow (e_1, \ldots, e_{g+1}) \\ \downarrow r:1 & E \to E \otimes \mathcal{O}_{\mathbb{P}^1}(g+1) \leftrightarrow L \\ \mathbb{P}^1 & (\lambda : 1) \in \mathbb{P}^1 \end{array}$$

Generalizations

- $\mathbb{P}^1 \to$ Riemann surface X of genus $g > 1$;
- E stable rank-r vector bundle over X. To give a concrete example, we will take $r=2$ and fix $\det E = \mathcal{O}_X$.

Hitchin's Abelianization Program

Fact (Hitchin). *Every such bundle E over X can be realized as the direct image of a line bundle over a spectral curve* $\Gamma \overset{r:1}{\to} X$.

We introduce the moduli space $\mathcal{M} = \mathcal{SU}_X(2, \mathcal{O}_X)$ = S-equivalence classes of E's, E semistable rank-2 bundle over X, $\det E = \mathcal{O}_X$. The dimension of $\mathcal{M}$ is $3g-3$.

Hitchin (1987) proved that $\mathcal{T}^*\mathcal{M}$ is ACI (generically, there exist $3g-3$ regular functions in involution with respect to the standard symplectic structure, with invariant manifolds isomorphic to Prym Γ, where Γ = spectral curve).

To recognize the analog of the features highlighted above, we recall that Kodaira–Spencer deformation theory gives the following description of the cotangent bundle: since a rank-r vector bundle over X is determined by a 1-cocycle with values in $\mathrm{GL}(r, \mathcal{O}_X)$, a first-order deformation of E is given by a 1-cocycle with values in the associated bundle of Lie algebras, hence by a class in $H^1(X, \mathrm{End}(E))$, so the cotangent bundle has Serre-dual fiber $H^0(X, E \otimes E^* \otimes K)$.

Hitchin map $(E, \phi) \in \mathcal{T}^*\mathcal{M}$ (Higgs field, trace zero, $\phi \in H^0(X, \mathrm{End}_0(E) \otimes K)$):

$H: \phi \mapsto \det\phi$ (more generally for any $r \geq 2$, $\mathrm{tr} \wedge^i \phi \in H^0(X, K^{\otimes i})$) $i = 2, \ldots, r$;

$\mu \mapsto -\mu$ defines Prym Γ, $\mu^2 = \det\phi \in H^0(X, K^{\otimes 2})$ defines Γ.

Explicit Hamiltonians for the Hitchin System

The cases in which X is genus 0 and 1 were solved explicitly by Nekrasov (1996) using explicit parametrizations of the moduli spaces; this includes the case of insertions (singular curves), yielding (elliptic) Gaudin models. We report the solution for the genus-2 case (van Geemen and Previato 1996).

Remark The map H projectivizes,

$$\bar{H} : \mathbb{P}H^0(X, \mathrm{End}_0(E) \otimes K) \to \mathbb{P}H^0(X, K^{\otimes 2})$$
$$\det(c\phi) = c^2 \det\phi$$

Coordinates on $\mathcal{T}^*\mathcal{M}$ can be given as follows:
$\Theta \subset \mathrm{Pic}^{g-1}X$ = canonical theta divisor

$$\Delta : \mathcal{M} \to |2\Theta| = \mathbb{P}^{2^g - 1}$$

$$E \mapsto D_E = \{\xi \in \mathrm{Pic}^{g-1}X : h^0(E \otimes \xi) > 0\}$$

X hyperelliptic $\Rightarrow \Delta$ is 2:1 except for $g=2$ (every point of $\mathcal{M}$ is fixed under the hyperelliptic

involution), where $\mathcal{M} \cong \mathbb{P}^3$. For a vector space V the Euler sequence gives

$$\mathbb{P}T^*\mathbb{P}V \cong I = \{(x,h) \in \mathbb{P}V \times \mathbb{P}V^* : x \in h\}$$

In our case,

$$\mathbb{P}V \times \mathbb{P}V^* = |2\Theta| \times |2\Theta_0|$$

Define six polynomial functions H_i on $\mathbb{P}^3 \times \mathbb{P}^{3*}$ by the requirement: for generic $q \in \mathbb{P}^3, (H_i = 0) \cap \mathbb{P}T_q\mathbb{P}^3 = \ell_i \cup \ell_i'$, the six pairs of bitangents to $\mathcal{K} \cap \mathbb{P}T_q^*\mathbb{P}^3$, where $\mathcal{K}$ is the Kummer surface (the remaining 16 bitangents are cut out by the tropes.)

Recall that the Grassmannian of lines in $\mathbb{P}^3, \mathrm{Gr}(2,4)$, is defined by an equation $\sum_1^6 X_i^2 = 0$ in Klein's coordinates

$$(X_1 : \ldots : X_6) \in \mathbb{P}^5$$

$$X_1 = p_{01} + p_{23}, \qquad X_2 = i(p_{01} - p_{23})$$

$$X_3 = i(p_{02} - p_{13}), \qquad X_4 = p_{02} + p_{13}$$

$$X_5 = p_{03} + p_{12}, \qquad X_6 = i(p_{03} - p_{12})$$

where $p_{ij} = Z_iW_j - W_jZ_i$ are Plücker's coordinates on the line

$$\langle (Z_0 : \ldots : Z_3)(W_0 : \ldots : W_3) \rangle \subseteq \mathbb{P}^{3*}$$

Using coordinates on the incidence variety I given by the sections Φ_i of the bundle projection $\mathbb{P}T^*\mathbb{P}^3 \to \mathbb{P}^3$, $\phi_i : \mathbb{P}^3 \to \mathbb{P}T^*\mathbb{P}^3 = I \subset \mathbb{P}^3 \times \mathbb{P}^{3*}, q \mapsto (q, \epsilon_i(q)) = (q, X_i(q, -))$, explicitly given, for $q = (x:y:z:t)$, by

$$\epsilon_1 = (y : -x : t : -z), \quad \epsilon_2 = (y : -x : -t : z)$$

$$\epsilon_3 = (z : t : -x : -y), \quad \epsilon_4 = (z : -t : -x : y)$$

$$\epsilon_5 = (t : z : -y : -x), \quad \epsilon_6 = (t : -z : y : -x)$$

$$x_j = X_j(\langle \epsilon_i(q), p \rangle)$$

Fact *For a point $q \in \mathbb{P}^3, p \in \mathbb{P}T_q^*\mathbb{P}^3, p \notin \epsilon_i(q)$, the ith Klein coordinate of the line $\langle \epsilon_i(q), p \rangle$ is zero and*

$$p \in \ell_i \cup \ell_i' \Leftrightarrow H_i(p,q) = \sum_{j \neq i} \frac{x_j^2}{\lambda_i - \lambda_j} = 0$$

with $x_j = X_j(\langle \epsilon_i(q), p \rangle)$.

Conclusion In an affine patch $\mathbb{C}^3 \times \mathbb{C}^{3*} \ni (q,p) = ((x:y:z:1), (u:v:w: -(xu + yv + zw)))$

$$H_i^a(p,q) = \sum_{j \neq i} \frac{X_j(\epsilon_i(q), p)^2}{\lambda_i - \lambda_j}$$

give six Hitchin Hamiltonians, any three of which are generically independent. The H_i^a have degree ≤ 4 in x, y, z and are homogeneous of degree 2 in u, v, w; they Poisson-commute with respect to $\mathrm{d}x \wedge \mathrm{d}u + \mathrm{d}y \wedge \mathrm{d}v + \mathrm{d}z \wedge \mathrm{d}w$.

Example An example is constituted by

$$\mu^2 = (\lambda^2 - 1)(\lambda^2 - 4)(\lambda^2 - 9)$$
$$((x:y:z:1), (u:v:w: -(xu + yv + zw)))$$
$$\in A^3 \times A^{3*}$$

$$\begin{aligned} H_1 = {} & uv(-70xy - 32x^3y - 18xy^3 - 10z - 32x^2z \\ & + 18y^2z) + v^2(-9 - 30y^2 - 16x^2y^2 - 9y^4 - 32xy^2 \\ & - 16z^2) + u^2(-16 - 40x^2 - 16x^4 - 9x^2y^2 + 18xyz \\ & - 9z^2) + vw(-18x + 10xy^2 + 10yz - 32x^2yz \\ & - 18y^3z - 32xz^2) + uw(32y + 10x^2y - 10xz \\ & - 32x^2z - 18xy^2z + 18yz^2) + w^2(-9x^2 - 16y^2 \\ & + 10xyz - 16x^2z^2 - 9y^2z^2) \end{aligned}$$

The concept of reduction and r-matrix have been generalized to Hitchin systems. Notably, Hitchin later showed that the Hamiltonians of the system appear as symbols of a heat operator that corresponds to a projectively flat connection, the quantization of the moduli space of bundles, obtained by changing the complex structure of the Riemann surface X.

Other Aspects

Special Functions

Special functions have also been traditionally significant in both algebraic geometry and integrable systems. Within the examples presented, elliptic functions gave rise to surprisingly sophisticated theories. The 1-wave solution encountered in the introduction, $u = 2\wp + \text{const.}$ in the limit when one or both periods of the Weierstrass function go to zero, becomes exponential or rational, respectively. The higher-genus analogs give rise to solitons, or rational solutions. On the other hand, the KP solutions which are doubly periodic in the x variable ("elliptic solitons") were classified by Krichever (cf. Dubrovin *et al.* (2001)), as forming an ACI Hamiltonian system ("elliptic Calogero–Moser"), which, 25 years later, is still generating important work, with Hamiltonian

$$H = \sum_{i=1}^{n} p_1^2 + \frac{1}{2} \sum_{i \neq j} \wp(q_i - q_j)$$

(where $\wp$ is the Weierstrass function of a lattice L with associated elliptic curve $X = \mathbb{C}/L$, $q \in X$ the origin) and $u = 2\sum_{i=1}^{n} \wp(x - x_i(t_2, t_3, \ldots))$ is a solution of the KP hierarchy for suitable time flows t_j of the system $(t_1 = x)$ and KP Baker function

$$\psi(x; \alpha) = \frac{\sigma(\alpha - x)}{\sigma(\alpha) - \sigma(x)} \mathrm{e}^{(\zeta(\alpha) \cdot x)}$$

The associated spectral curves have been classified in moduli by Treibich and Verdier (cf. Treibich (2001)); Krichever produced a two-field model as

well as a universal Poisson structure for the system; Donagi and Markman (1996) realized it as a generalized Hitchin system.

More classically, elliptic potentials were the subject of much study, in particular by Lamé and Hermite in the nineteenth century and Ince in the twentieth; a sample result due to Ince makes one feel like Alice in Wonderland, who "knelt down and looked along the passage into the loveliest garden you ever saw": the Lamé operator $L = -\partial^2 + a(a+1)\wp(x - x_0)$ with real, smooth potential is finite gap (namely, almost all the periodic eigenvalues are double) iff $a \in \mathbb{Z}$ (if a is positive the number of gaps is a). A generalization to several variables (due to Chalykh and Veselov),

$$L = -\Delta + \sum_{\alpha \in R_+} g_\alpha \wp(\langle \alpha, x \rangle)$$

where R_+ is the set of positive roots for a simple complex Lie algebra of rank n, $\langle -, - \rangle$ is some scalar product in $\mathbb{R}^n$, invariant under the action of the Weyl group, and $g_\alpha = m_\alpha(m_\alpha + 1)\langle \alpha, \alpha \rangle$ for some $m_\alpha \in \mathbb{Z}$, provides one of the few known examples of quantum completely integrable rings of differential operators in several variables. Roughly speaking, this means that the centralizer of L contains n operators with functionally independent symbols, where n is the number of variables.

What is more, Chalykh *et al.* (2003) combine differential Galois theory and elliptic function theory to characterize (under some mild assumptions) the generalized Lamé operators that are algebraically completely integrable: the differential Galois group of the solutions is abelian.

Duality, Fourier–Mukai Transform, and Bispectrality

Duality is a concept imported from mathematical physics; as a mathematical phenomenon, it has not reached theoretical maturity. First observed in examples, as in Fock *et al.* (2000), where different definitions of dual ACI Hamiltonian systems were given (action-angle, action–action, and quantum), it resurfaced for the Hitchin system, in more than one guise, whether it be an interchange of position and momentum variables (Gawędzki and Tran-Ngoc-Bich 1998) or a duality between the Lagrangian tori that fiber two such systems, coming from a Fourier–Mukai transform, namely a twist by the (universal) Picard line bundle:

$$\begin{array}{c} \mathcal{P} \\ \downarrow \\ \mathrm{Jac}(X) \times (H^0(X, K) = T^*\mathrm{Jac}(X)) \end{array}$$

Notably, the Picard bundle was used by Nakayashiki to give a spectacular generalization of the Burchnall–Chaundy result for a genus-2 curve X (more generally, $\mathrm{Jac}(X)$ is replaced by a generic abelian variety in the statement): the coordinate ring of $\mathrm{Jac}(X) - \Theta_X$ is the common spectrum of a ring of commuting $(g! \times g!)$ matrix partial differential operators in g variables. The Fourier transform allowed him to extend Sato's correspondence $\partial^{-1} \leftrightarrow z$ and give $\mathcal{F}$ a unique (free, rank-$g!$) $D_{\mathrm{Jac}(X)}$-module structure, where $\mathcal{F}$ is a suitable coherent sheaf over $\mathrm{Jac}(X)$ generalizing the Baker function.

In this model, the interchange of the x and z variables is known as bispectrality (cf. Grünbaum (2001)): a somewhat narrower question is a characterization of the differential operators L in x for which there exists a differential operator B in k and a common eigenfunction:

$$\begin{cases} L\psi(x,k) = f(k)\psi(x,k) \\ B\psi(x,k) = \theta(x)\psi(x,k) \end{cases}$$

for some functions f, θ, typically polynomial. This question proved to be related with the KP hierarchy and isomonodromy deformations. When to a hierarchy there is associated an ACI Hamiltonian system (as in the Neumann case shown above), bispectrality may produce a dual system, in a sense related to the ones discussed, but somewhat mysteriously so.

Conclusion

Many important mathematical topics and individual contributions regrettably have to go unmentioned in an article of this length. The aim was to illustrate by simplest examples the geometric nature of integrable systems and equations, in the areas of spectral curves, moduli of vector bundles over them, Grassmann manifolds, special functions, Poisson geometry, representation theory, as well as mention constructions that are not yet complete, such as spectral varieties of higher dimension, dualities sweeping vaster moduli spaces, and quantization.

See also: Billiards in bounded convex domains; $\bar{\partial}$-Approach to Integrable Systems; Functional Equations and Integrable Systems; Integrable Systems and Discrete Geometry; Integrable Systems and Recursion Operators on Symplectic and Jacobi Manifolds; Integrable Systems and the Inverse Scattering Method; Integrable Systems in Random Matrix Theory; Integrable Systems: Overview; Multi-Hamiltonian Systems; Recursion Operators in Classical Mechanics; Riemann–Hilbert Methods in Integrable Systems; Solitons and Kac–Moody Lie Algebras.

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Integrable Systems and Discrete Geometry

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Introduction

Although the main subject of this article is the connection between integrable discrete systems and geometry, we feel obliged to begin with the differential part of the relation.

Classical Differential Geometry and Integrable Systems

The oldest (1840) integrable nonlinear partial differential equation recorded in literature is the Lamé system

$$\frac{\partial^2 H_i}{\partial u_j \partial u_k} - \frac{1}{H_j}\frac{\partial H_j}{\partial u_k}\frac{\partial H_i}{\partial u_j} - \frac{1}{H_k}\frac{\partial H_k}{\partial u_j}\frac{\partial H_i}{\partial u_k} = 0, \quad i,j,k \text{ distinct} \qquad [1]$$

$$\frac{\partial}{\partial u_k}\left(\frac{1}{H_k}\frac{\partial H_j}{\partial u_k}\right) + \frac{\partial}{\partial u_j}\left(\frac{1}{H_j}\frac{\partial H_k}{\partial u_j}\right) + \frac{1}{H_i^2}\frac{\partial H_j}{\partial u_i}\frac{\partial H_k}{\partial u_i} = 0 \qquad [2]$$

describing orthogonal coordinates in the three-dimensional Euclidean space $\mathbb{E}^3$ (indices i,j,k range from 1 to 3). Already in 1869, it was found by Ribaucour that the nonlinear Lamé system possesses a discrete symmetry enabling to construct, in a linear way, new solutions of the system from the old ones. He gave also a geometric interpretation of this symmetry in terms of certain spheres tangent to the coordinate surfaces of the triply orthogonal system. In 1918, Bianchi showed that the result of superposition of the Ribaucour transformations is, in a certain sense, independent of the order of their composition.

Such properties of a nonlinear equation are hallmarks of its integrability, and indeed, the Lamé system was solved using soliton techniques in 1997–98. The above example illustrates the close connection between the modern theory of integrable partial differential equations and the differential geometry of the turn of the nineteenth and twentieth centuries. A remarkable property of certain parametrized submanifolds (and then of the corresponding equations) studied that time is that they allow for transformations which exhibit the so-called "Bianchi permutability property." Such transformations called, depending on the context, the Darboux, Calapso, Christoffel, Bianchi, Bäcklund, Laplace,

Koenigs, Moutard, Combescure, Lévy, Goursat, Ribaucour, or the fundamental transformation of Jonas, can be geometrically described in terms of certain families of lines called line congruences.

In the connection between integrable systems and differential geometry, a distinguished role is played by the multidimensional conjugate nets, described by the Darboux system, which is just the first part [1] of the Lamé system with indices ranging form 1 to $N \geq 3$. On the level of integrable systems, this dominant role has the following explanation: the Darboux system, together with equations describing isoconjugate deformations of the net, forms the multicomponent Kadomtsev–Petviashvilii (KP) hierarchy, which is viewed as a master system of equations in soliton theory. In fact, in appropriate variables, the whole multicomponent KP hierarchy can be rewritten as an infinite system of the Darboux equations.

Transition to the Discrete Domain

The recent progress in studying discrete integrable systems showed that, in many respects, they should be considered as more fundamental than their differential counterparts. Consequently, the natural problem of extending the geometric interpretation of integrable partial differential equations to the discrete domain arose, leading not only to the transition to the discrete domain of many results on the connection between the differential geometry and integrable systems, but also – and this seems to be even more important – to the description of integrability in a very elementary and purely geometric way.

At the level of integrable equations, the transition "from differential to discrete" often makes formulas more complicated and longer. On the contrary, at the geometric level, in such a transition the properties of discrete submanifolds, relevant to their integrability, become simpler and more transparent. Indeed, the mathematics necessary to understand the basic ideas of the integrable discrete geometry does not exceed the "ruler and compass constructions," and many proofs can be performed using elementary incidence geometry.

We will concentrate our attention on the multidimensional lattice made from planar quadrilaterals, which is the discrete analog of a conjugate net. Together with the discussion of its properties, which are the core of the geometric integrability, we briefly present the analytic methods of construction of these lattices and we also describe some basic multidimensional integrable reductions of them. Then we discuss integrable discrete surfaces; some of them have been found in the early period of the "case-by-case" studies. We shall however try to present them, from a unifying perspective, as reductions of the quadrilateral lattice (QL).

Multidimensional Integrable Lattices

The Quadrilateral Lattice

An N-dimensional lattice $\boldsymbol{x}:\mathbb{Z}^N \to \mathbb{R}^M$ is a lattice made from planar quadrilaterals, or a quadrilateral lattice (QL) in short, if its elementary quadrilaterals $\{\boldsymbol{x}, T_i\boldsymbol{x}, T_j\boldsymbol{x}, T_iT_j\boldsymbol{x}\}$ are planar; that is, iff the following system of discrete Laplace equations is satisfied:

$$\Delta_i\Delta_j\boldsymbol{x} = (T_iA_{ij})\Delta_i\boldsymbol{x} + (T_jA_{ji})\Delta_j\boldsymbol{x}, \quad i \neq j, \; i,j = 1,\ldots,N \qquad [3]$$

where $A_{ij}:\mathbb{Z}^N \to \mathbb{R}$ are functions of the discrete variable; here T_i is the translation operator in the ith direction, and $\Delta_i = T_i - 1$ is the corresponding difference operator. For simplicity, we work here in the affine setting neglecting projective geometric aspects of the theory.

The geometric integrability scheme In the case $N=2$ the definition [3] allows one to uniquely construct, given two discrete curves intersecting in a common vertex and two functions $A_{12}, A_{21} : \mathbb{Z}^2 \to \mathbb{R}$, a quadrilateral surface. For $N > 2$ the planarity constraints [3] are instead compatible if and only if the geometric data A_{ij} satisfy the nonlinear system

$$\begin{aligned} &\Delta_k A_{ij} + (T_k A_{ij})A_{ik} \\ &\quad = (T_j A_{jk})A_{ij} + (T_k A_{kj})A_{ik} \\ &\quad\quad i,j,k \quad \text{distinct} \end{aligned} \qquad [4]$$

This constraint has a very simple interpretation: in building the elementary cube (see **Figure 1**), the seven points $\boldsymbol{x}, T_i\boldsymbol{x}, T_j\boldsymbol{x}, T_k\boldsymbol{x}, T_iT_j\boldsymbol{x}, T_iT_k\boldsymbol{x}$, and $T_jT_k\boldsymbol{x}$ (i,j,k are distinct) determine the eighth point $T_iT_jT_k\boldsymbol{x}$ as the unique intersection of three planes in the three-dimensional space.

The connection of this elementary geometric point of view with the classical theory of integrable systems is transparent: the planarity constraint corresponds to the set of linear spectral problems [3] and the resulting QL is characterized by the nonlinear equations [4], arising as the compatibility conditions for such spectral problems. Since the QL equations [4] are a master system in the theory of integrable equations, planarity can be viewed as the elementary geometric root of integrability. The idea

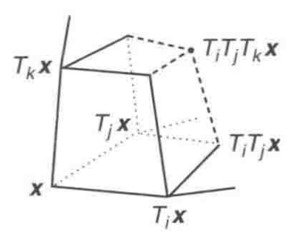


Figure 1 The geometric integrability scheme.

that integrability be associated with the consistency of a geometric (and/or algebraic) property when increasing the dimensionality of the system is recurrent in the theory of integrable systems.

Other forms of the Darboux system The $i \leftrightarrow j$ symmetry of the RHS of eqns [4] implies the existence of the potentials $H_i : \mathbb{Z}^N \to \mathbb{R}$ (the Lamé coefficients) such that

$$A_{ij} = \frac{\Delta_j H_i}{H_i}, \quad i \neq j \qquad [5]$$

and then eqns [4] take the form

$$\Delta_k \Delta_j H_i - \left(T_j \frac{\Delta_k H_j}{H_j}\right) \Delta_j H_i - \left(T_k \frac{\Delta_j H_k}{H_k}\right) \Delta_k H_i = 0, \quad i,j,k \text{ distinct} \qquad [6]$$

which is the discrete version of the first part [1] of the Lamé system.

The Lamé coefficients allow to define the suitably normalized tangent vectors $\boldsymbol{X}_i : \mathbb{Z}^N \to \mathbb{R}^M$ by equations

$$\Delta_i \boldsymbol{x} = (T_i H_i) \boldsymbol{X}_i \qquad [7]$$

and the functions $Q_{ij} : \mathbb{Z}^N \to \mathbb{R}, i \neq j$, (the rotation coefficients) by equations

$$\Delta_i H_j = (T_i H_i) Q_{ij}, \quad i \neq j \qquad [8]$$

Then eqns [3] and [6] can be rewritten in the first-order form

$$\Delta_j \boldsymbol{X}_i = (T_j Q_{ij}) \boldsymbol{X}_j, \quad i \neq j \qquad [9]$$

$$\Delta_k Q_{ij} = (T_k Q_{ik}) Q_{kj}, \quad i,j,k \text{ distinct} \qquad [10]$$

The discrete Darboux system [10] implies the existence of other potentials ρ_i defined by the compatible equations

$$\frac{T_j \rho_i}{\rho_i} = 1 - (T_i Q_{ji})(T_j Q_{ij}), \quad i \neq j \qquad [11]$$

The $i \leftrightarrow j$ symmetry of the RHS of eqns [11] implies the existence of yet another potential $\tau : \mathbb{Z}^N \to \mathbb{R}$,

$$\rho_i = \frac{T_i \tau}{\tau} \qquad [12]$$

which is called the τ-function of the QL. In terms of the τ-function, and of the functions

$$\tau_{ij} = \tau Q_{ij}, \quad i \neq j \qquad [13]$$

whose geometric interpretation will be given in a later section, the discrete Darboux equations take the following Hirota-type form:

$$(T_i T_j \tau)\tau = (T_i \tau) T_j \tau - (T_i \tau_{ji}) T_j \tau_{ij}, \quad i \neq j \qquad [14]$$

$$(T_k \tau_{ij})\tau = (T_k \tau)\tau_{ij} + (T_k \tau_{ik})\tau_{kj}, \quad i, j, k \text{ distinct} \qquad [15]$$

Analytic Methods

We will show how one can construct large classes of solutions of the discrete Darboux equations and the corresponding QLs using two basic analytical methods of the soliton theory: the $\bar\partial$-dressing method and the algebro-geometric techniques.

The $\bar\partial$-dressing method Consider the nonlocal $\bar\partial$-problem

$$\begin{gathered} \bar\partial \chi(z) + (\hat{R}\chi)(z) = \bar\partial \nu(z) \\ \lim_{|z| \to \infty} (\chi(z) - \nu(z)) = 0 \end{gathered} \qquad [16]$$

where $\bar\partial = \partial / \partial \bar z$, $\hat R$ is the integral operator

$$(\hat R \chi)(z) = \int_{\mathbb{C}} R(z, z') \chi(z') \, dz' \wedge d\bar z'$$

and $\nu(z)$ is a given rational function of z.

Let $Q_i^{\pm} \in \mathbb{C}, i = 1, \ldots, N$ be pairs of distinct points of the complex plane, which define the dependence of the kernel R on the discrete variable $n \in \mathbb{Z}^N$:

$$R(z, z'; n) = \prod_{i=1}^{N} \left(\frac{z - Q_i^+}{z - Q_i^-}\right)^{n_i} \times R_0(z, z') \prod_{i=1}^{N} \left(\frac{z' - Q_i^-}{z' - Q_i^+}\right)^{n_i}$$

We consider only kernels $R_0(z, z')$ such that the nonlocal $\bar\partial$-problem is uniquely solvable. If $\chi(z; n)$ is the unique solution with the canonical normalization $\nu = 1$, then the function

$$\psi(z; n) = \chi(z; n) \prod_{i=1}^{N} \left(\frac{z - Q_i^-}{z - Q_i^+}\right)^{n_i}$$

satisfies the system of the Laplace equations [3] with the Lamé coefficients given by

$$H_i(n) = \lim_{z \to Q_i^+} \left(\left(\frac{z - Q_i^+}{z - Q_i^-}\right)^{n_i} \psi(z; n) \right)$$

By construction, the system of such Laplace equations is compatible, therefore the Lamé coefficients satisfy eqns [6]. To various n-independent measures $d\mu_a$ on $\mathbb{C}$ there correspond coordinates

$$x^a(n) = \int_{\mathbb{C}} \psi(z; n) \, d\mu_a(z)$$

of a QL $\boldsymbol{x}$, having $H_i(n)$ as the Lamé coefficients. To have real lattices, the kernel R_0, the points $Q_i^{\pm}$, and the measures $d\mu_a$ should satisfy certain additional conditions.

One can find a similar interpretation of the normalized tangent vectors $\boldsymbol{X}_i$ and of the rotation

coefficients Q_{ij}. If $\chi_i(z;n)$ are the unique solutions of the nonlocal $\bar{\partial}$-problem [16] with the normalizations

$$\nu_i(z;n) = \left(\frac{Q_i^+ - Q_i^-}{z - Q_i^+}\right) \prod_{k=1,k\neq i}^{N} \left(\frac{Q_i^+ - Q_k^+}{Q_i^+ - Q_k^-}\right)^{n_k}$$

then the functions $\psi_i(z;n)$, defined by

$$\psi_i(z;n) = \prod_{k=1}^{N} \left(\frac{z - Q_k^-}{z - Q_k^+}\right)^{n_k} \chi_i(z;n)$$

satisfy the direct analog of the linear problem [9],

$$\Delta_j \psi_i(z;n) = (T_j Q_{ij}(n))\psi_j(z;n), \quad i \neq j \qquad [17]$$

where

$$Q_{ij}(n) = \lim_{z\to Q_j^+} \left(\left(\frac{z - Q_j^+}{z - Q_j^-}\right)^{n_j} \psi_i(z;n) \right)$$

Again, by construction, eqns [17] are compatible and the functions $Q_{ij}(n)$ satisfy the discrete Darboux equations [10]. The functions

$$X_i^a(n) = \int_{\mathbb{C}} \psi_i(z;n)\, \mathrm{d}\mu_a(z)$$

are coordinates of the normalized tangent vectors $\boldsymbol{X}_i$ of the QL $\boldsymbol{x}$ constructed above.

The algebro-geometric techniques Given a compact Riemann surface $\mathcal{R}$ of genus g, consider a nonspecial divisor $D = \sum_{\alpha=1}^{g} P_\alpha$. Choose N pairs of points $Q_i^\pm \in \mathcal{R}$ and the normalization point Q_∞. Given $n \in \mathbb{Z}^N$, there exists a unique Baker–Akhiezer function $\psi(n)$, defined as a meromorphic function on $\mathcal{R}$, with the following analytical properties: (1) as a function of $P \in \mathcal{R} \setminus \cup_{i=1}^{N} Q_i^\pm$, $\psi(n)$ may have as singularities only simple poles in the points of the divisor D; (2) in the points $Q_i^\pm$ function $\psi(n)$ has poles of the order $\pm n_i$; and (3) in the point Q_∞ function $\psi(n)$ is normalized to 1.

When $z_i^\pm(P)$ is a local coordinate on $\mathcal{R}$ centered at $Q_i^\pm$, then condition (2) implies that the function $\psi(n)$ in a neighborhood of the point $Q_i^\pm$ is of the form

$$\psi(P;n) = \left(z_i^\pm(P)\right)^{\mp n_i} \left(\sum_{s=0}^{\infty} \xi_{s,\pm}^i(n) \left(z_i^\pm(P)\right)^s \right) \qquad [18]$$

The Baker–Akhiezer function, as a function of the discrete variable $n \in \mathbb{Z}^N$, satisfies the system of Laplace equations [3] with the Lamé coefficients $H_i(n) = \xi_{0,+}^i(n)$.

Again, by construction, the Lamé coefficients satisfy eqns [6]. To various n-independent measures $\mathrm{d}\mu_a$ on $\mathcal{R}$ there correspond coordinates

$$x^a(n) = \int_{\mathcal{R}} \psi(P;n)\, \mathrm{d}\mu_a(P)$$

of a QL $\boldsymbol{x}$.

We present the expression of the Baker–Akhiezer function and of the τ-function of the QL in terms of the Riemann theta functions. Let us choose on $\mathcal{R}$ the canonical basis of cycles $\{a_1, \ldots, a_g, b_1, \ldots, b_g\}$ and the dual basis $\{\omega_1, \ldots, \omega_g\}$ of holomorphic differentials on $\mathcal{R}$, that is, $\oint_{a_j} \omega_k = \delta_{jk}$. Then the matrix B of b-periods defined as $B_{jk} = \oint_{b_j} \omega_k$ is symmetric and has positively defined imaginary part. Denote by ω_{PQ} the unique differential holomorphic in $\mathcal{R}\setminus\{P, Q\}$ with poles of the first order in P, Q and residues, correspondingly, 1 and -1, which is normalized by conditions $\oint_{a_j} \omega_{PQ} = 0$. The Riemann function $\theta(z;B), z \in \mathbb{C}^g$, is defined by its Fourier expansion

$$\theta(z;B) = \sum_{m\in\mathbb{Z}^g} \exp\{\pi \mathrm{i}\langle m, Bm\rangle + 2\pi\mathrm{i}\langle m, z\rangle\}$$

where $\langle\cdot,\cdot\rangle$ denotes the standard bilinear form in $\mathbb{C}^g$. Finally, the Abel map A is given by $A(P) = (\int_{P_0}^{P} \omega_1, \ldots, \int_{P_0}^{P} \omega_g)$, where $P_0 \in \mathcal{R}$, and the Riemann constants vector K is given by

$$K_j = \frac{1 + B_{jj}}{2} - \sum_{k\neq j} \left(\oint_{a_k} \omega_k(P) A_j(P) \omega_j \right),$$
$$j = 1, \ldots, g$$

The explicit form of the vacuum Baker–Akhiezer function ψ can be written down with the help of the theta functions as follows:

$$\psi(n,P) = \frac{\theta\left(A(P) + \sum_{k=1}^{N} n_k (A(Q_k^-) - A(Q_k^+)) + Z\right)}{\theta\left(A(Q_\infty) + \sum_{k=1}^{N} n_k (A(Q_k^-) - A(Q_k^+)) + Z\right)} \times \frac{\theta(A(Q_\infty) + Z)}{\theta(A(P) + Z)} \exp\left(\sum_{k=1}^{N} n_k \int_{Q_\infty}^{P} \omega_{Q_k^- Q_k^+} \right)$$

where $Z = -\sum_{j=1}^{g} A(P_j) - K$.

Denote by $r_{kj}^\pm$ and $s_{kj}^\pm$ the constants in the decomposition of the abelian integrals near the point $Q_j^\pm$

$$\int_{P_0}^{P} \omega_{Q_k^- Q_k^+} \overset{P\to Q_j^\pm}{=} \mp\delta_{kj} \log z_j^\pm(P) + r_{kj}^\pm + O\left(z_j^\pm(P)\right)$$

$$\int_{P_0}^{P} \omega_{Q_\infty Q_k^+} \overset{P\to Q_j^\pm}{=} -\delta_{kj}\delta_{+\pm} \log z_j^\pm(P) + s_{kj}^\pm + O\left(z_j^\pm(P)\right)$$

Then the expression of the τ-function of the QL within the subclass of algebro-geometric solutions reads

$$\tau(n) = \theta\left(\sum_{k=1}^{N} n_k (A(Q_k^-) - A(Q_k^+)) + A(Q_\infty) + Z \right) \times \prod_{k,j=1}^{N} \lambda_{kj}^{n_k n_j} \prod_{k=1}^{N} \mu_k^{n_k}$$

where

$$\lambda_{kj} = \exp\left(\frac{r_{kj}^{-} - r_{kj}^{+}}{2}\right) = \lambda_{jk}$$

$$\mu_k = \frac{1}{\lambda_{kk}} \frac{\theta(A(Q_k^{+}) + Z)}{\theta(A(Q_k^{-}) + Z)} \exp(s_{kk}^{-} - s_{kk}^{+})$$

Finally, we remark that the geometric integrability scheme and the algebro-geometric methods work also in the finite fields setting, giving solutions of the corresponding integrable cellular automata.

The Darboux-Type Transformations

We present the basic ideas and results of the theory of the Darboux-type transformations of the multidimensional QL.

Line congruences and the fundamental transformation
To define the transformations we need to define first N-dimensional line congruences (or, simply, congruences), which are families of lines in $\mathbb{R}^M$ labeled by points of $\mathbb{Z}^N$ with the property that any two neighboring lines $\mathfrak{l}$ and $T_i\mathfrak{l}, i = 1, \ldots, N$, are coplanar and therefore (eventually in the projective extension $\mathbb{P}^M$ of $\mathbb{R}^M$) intersect.

The QL $\mathcal{F}(\boldsymbol{x})$ is a fundamental transform of the QL $\boldsymbol{x}$ if the lines connecting the corresponding points of the lattices form a congruence. The superposition of a number of fundamental transformations can be compactly formulated in the vectorial fundamental transformation. The data of the vectorial fundamental transformation are: (1) the solution $\boldsymbol{Y}_i : \mathbb{Z}^N \to \mathbb{V}$, $\mathbb{V}$ being a linear space, of the linear system [9]; (2) the solution $\boldsymbol{Y}_i^* : \mathbb{Z}^N \to \mathbb{V}^*$, $\mathbb{V}^*$ being the dual of $\mathbb{V}$, of the linear system [8]. These allow to construct the linear operator-valued potential $\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*) : \mathbb{Z}^N \to L(\mathbb{V})$, defined by the following analog of eqn [7]:

$$\Delta_i \boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*) = \boldsymbol{Y}_i \otimes (T_i \boldsymbol{Y}_i^*), \quad i = 1, \ldots, N \qquad [19]$$

Similarly, one defines $\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*) : \mathbb{Z}^N \to L(\mathbb{V}, \mathbb{R}^M)$ and $\boldsymbol{\Omega}(\boldsymbol{Y}, H) : \mathbb{Z}^N \to \mathbb{V}$. The transforms of the lattice $\boldsymbol{x}$ and other related functions are given by

$$\mathcal{F}(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*)\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{-1}\boldsymbol{\Omega}(\boldsymbol{Y}, H)$$

$$\mathcal{F}(H_i) = H_i - \boldsymbol{Y}_i^*\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{-1}\boldsymbol{\Omega}(\boldsymbol{Y}, H), \quad i = 1, \ldots, N$$

$$\mathcal{F}(\boldsymbol{X}_i) = \boldsymbol{X}_i - \boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*)\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{-1}\boldsymbol{Y}_i, \quad i = 1, \ldots, N$$

$$\mathcal{F}(Q_{ij}) = Q_{ij} - \boldsymbol{Y}_j^*\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{-1}\boldsymbol{Y}_i, \quad i,j = 1, \ldots, N, \ i \neq j$$

$$\mathcal{F}(\rho_i) = \rho_i(1 + (T_i\boldsymbol{Y}_i^*)\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)\boldsymbol{Y}_i), \quad i = 1, \ldots, N$$

$$\mathcal{F}(\tau) = \tau \det \boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)$$

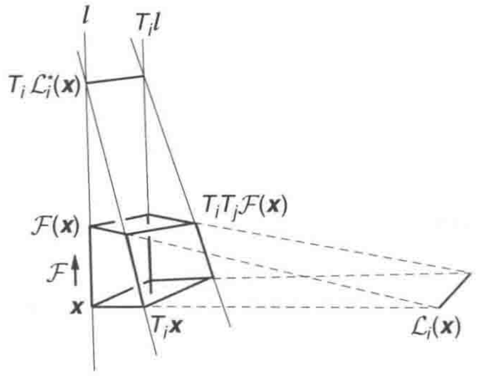


Figure 2 The fundamental transformation as the binary transformation.

Notice that, by the coplanarity of any two neighboring lines of the congruence, also the quadrilaterals $\{\boldsymbol{x}, T_i\boldsymbol{x}, \mathcal{F}(\boldsymbol{x}), \mathcal{F}(T_i\boldsymbol{x})\}$ are planar (see **Figure 2**). Then the construction of the transformed lattice mimics the geometric integrability scheme. In consequence, any quadrilateral

$$\{\boldsymbol{x}, \mathcal{F}_1(\boldsymbol{x}), \mathcal{F}_2(\boldsymbol{x}), \mathcal{F}_1(\mathcal{F}_2(\boldsymbol{x})) = \mathcal{F}_2(\mathcal{F}_1(\boldsymbol{x}))\}$$

is planar as well. Therefore, on the discrete level, there is no difference between the lattice coordinate directions and the fundamental transformation directions. The distinction becomes visible in the limit from the QL to the conjugate net. Therefore, the vectorial description of the superposition of the fundamental transformations not only implies their permutability but also provides the explanation of the validity of the practical rule of "integrable discretization by Darboux transformations."

The Lévy and Combescure transformations It is easy to see that the family $\mathfrak{t}_i$ of lines passing through the points $\boldsymbol{x}$ and $T_i\boldsymbol{x}$ of a QL forms a congruence, called the ith tangent congruence of the lattice. When the congruence of the transformation is the ith tangent congruence of the lattice $\boldsymbol{x}$, then the corresponding reduction of the fundamental transformation is called the "Lévy transformation" $\mathcal{L}_i$.

It turns out that, for a generic congruence $\mathfrak{l}$, the lattice made from intersection points of the lines $\mathfrak{l}$ and $T_i^{-1}\mathfrak{l}$ is a QL, called the ith focal lattice of the congruence. When the fundamental transform of the lattice $\boldsymbol{x}$ is the ith focal lattice of the transformation congruence, then the corresponding reduction of the fundamental transformation is called the "adjoint Lévy transformation" $\mathcal{L}_i^*$.

Both Lévy transformations use only a half of the fundamental transformation data, and the corresponding reduction formulas (in the scalar case) for the lattice points read as follows:

$$\mathcal{L}_i(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{X}_i(Y_i)^{-1}\boldsymbol{\Omega}(Y, H)$$

$$\mathcal{L}_i^*(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{\Omega}(\boldsymbol{X}, Y^*)\,(Y_i^*)^{-1}H_i$$

Notice that the composition of the Lévy and the adjoint Lévy transformations gives (see **Figure 2**) the fundamental transformation, also called, for this reason, the binary transformation.

Another reduction of the fundamental transformation, important from a technical point of view, is the "Combescure transformation," in which the tangent lines of the transformed lattice $\mathcal{C}(\boldsymbol{x})$ are parallel to those of the lattice $\boldsymbol{x}$. The transformation formula reads

$$\mathcal{C}(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{\Omega}(\boldsymbol{X}, Y^*)$$

where only the solution Y^* of the adjoint linear system [8], necessary to build the transformation congruence, is needed.

The Laplace transformations and the geometric meaning of the Hirota equation The Laplace transform $\mathcal{L}_{ij}(\boldsymbol{x}), i \neq j$, of the QL $\boldsymbol{x}$ is the jth focal lattice of its ith tangent congruence (see **Figure 3**). It is uniquely determined once the lattice $\boldsymbol{x}$ is given. The transformation formulas of the lattice points and of the τ-function read as follows:

$$\mathcal{L}_{ij}(\boldsymbol{x}) = \boldsymbol{x} - \frac{1}{A_{ji}}\Delta_i \boldsymbol{x} \qquad [20]$$

$$\mathcal{L}_{ij}(\tau) = \tau_{ij} = \tau Q_{ij} \qquad [21]$$

The superpositions of Laplace transformations satisfy the following identities

$$\mathcal{L}_{ij} \circ \mathcal{L}_{ji} = \mathrm{id}$$
$$\mathcal{L}_{jk} \circ \mathcal{L}_{ij} = \mathcal{L}_{ik}$$
$$\mathcal{L}_{ki} \circ \mathcal{L}_{ij} = \mathcal{L}_{kj}$$

which allow to identify them with the Schlesinger transformations of the monodromy theory.

In the simplest case $N=2$ one obtains the so-called Laplace sequence of two-dimensional QLs

$$\boldsymbol{x}_\ell = \mathcal{L}_{12}^\ell(\boldsymbol{x}), \qquad \tau_\ell = \mathcal{L}_{12}^\ell(\tau)$$
$$\mathcal{L}_{12}^{-1} = \mathcal{L}_{21}, \quad \ell \in \mathbb{Z}$$

Equations [14] and [21] imply that the τ-functions of the Laplace sequence satisfy the celebrated Hirota equation (the fully discrete Toda system)

$$\tau_\ell T_1 T_2 \tau_\ell = (T_1\tau_\ell)(T_2\tau_\ell) - (T_1\tau_{\ell-1})(T_2\tau_{\ell+1})$$

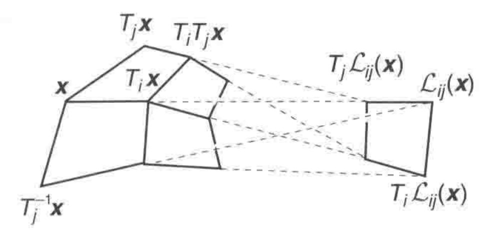


Figure 3 The Laplace transformation $\mathcal{L}_{ij}$.

Distinguished Integrable Reductions

We will present here basic reductions of the multidimensional QL. The geometric criterion for their integrability is the compatibility with the geometric integrability scheme.

The circular lattices and the Ribaucour congruences QLs $\mathbb{Z}^N \to \mathbb{E}^M$ for which each quadrilateral is inscribed in a circle are called "circular" lattices. They are the integrable discrete analogs of submanifolds parametrized by curvature coordinates (e.g., the orthogonal coordinate systems described by the Laméequations [1]–[2]).

The integrability of circular lattices is the consequence of the fact that if the three "initial" quadrilaterals $\{\boldsymbol{x}, T_i\boldsymbol{x}, T_j\boldsymbol{x}, T_iT_j\boldsymbol{x}\}$, $\{\boldsymbol{x}, T_i\boldsymbol{x}, T_k\boldsymbol{x}, T_iT_k\boldsymbol{x}\}$, $\{\boldsymbol{x}, T_j\boldsymbol{x}, T_k\boldsymbol{x}, T_jT_k\boldsymbol{x}\}$ are circular, then also the three new quadrilaterals constructed by adding the vertex $T_iT_jT_k\boldsymbol{x}$ are circular as well (see **Figure 4**). In fact, all the eight vertices belong to a sphere, and, in consequence, all the vertices of any K-dimensional, $K = 2, \ldots, N$, elementary cell belong to a $(K-1)$-dimensional sphere.

There are various equivalent algebraic descriptions of the circular lattices:

1. the normalized tangent vectors $\boldsymbol{X}_i$ satisfy the constraint
$$\boldsymbol{X}_i \cdot T_i\boldsymbol{X}_j + \boldsymbol{X}_j \cdot T_j\boldsymbol{X}_i = 0, \quad i \neq j$$
2. the scalar function $\boldsymbol{x}\cdot\boldsymbol{x}: \mathbb{Z}^N \to \mathbb{R}$ satisfies the Laplace equations [3] of the lattice $\boldsymbol{x}$;
3. the functions $X_i^\circ = (\boldsymbol{x} + T_i\boldsymbol{x}) \cdot \boldsymbol{X}_i : \mathbb{Z}^N \to \mathbb{R}$ satisfy the same linear system [9] as the normalized tangent vectors $\boldsymbol{X}_i$; and
4. the functions $\boldsymbol{X}_i \cdot \boldsymbol{X}_i : \mathbb{Z}^N \to \mathbb{R}$ satisfy eqns [11] and thus can serve as the potentials ρ_i.

The Ribaucour transformation $\mathcal{R}$ is the restriction of the fundamental transformation to the class of circular lattices such that also the "side" quadrilaterals $\{\boldsymbol{x}, T_i\boldsymbol{x}, \mathcal{R}(\boldsymbol{x}), \mathcal{R}(T_i\boldsymbol{x})\}$ are circular. Again there is no geometric difference between the lattice directions and the Ribaucour transformation direction. Moreover, the quadrilaterals $\{\boldsymbol{x}, \mathcal{R}_1(\boldsymbol{x}),$

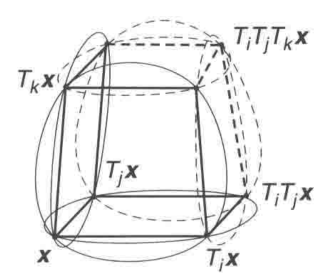


Figure 4 The geometric integrability of circular lattices.

$\mathcal{R}_2(\boldsymbol{x}), \mathcal{R}_1(\mathcal{R}_2(\boldsymbol{x})) = \mathcal{R}_2(\mathcal{R}_1(\boldsymbol{x}))\}$ are circular as well. In consequence, the vertices of the elementary K-cells, $K = 2, \ldots, N$, of the circular lattice and the corresponding vertices of its Ribaucour transform are contained in a K-dimensional sphere. Finally, for $K = N$, one obtains a special $\mathbb{Z}^N$ family of N-dimensional spheres, called the Ribaucour congruence of spheres.

Algebraically, the Ribaucour transformation needs only a half of the data (necessary to build the congruence) of the fundamental transformation. The data of the vectorial Ribaucour transformation consists of the solution $\boldsymbol{Y}_i^* : \mathbb{Z}^N \to \mathbb{V}^*$, of the linear system [8]. Then, because of the circularity constraint, $\boldsymbol{Y}_i : \mathbb{Z}^N \to \mathbb{V}$ given by

$$\boldsymbol{Y}_i = (\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*) + T_i\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*))^{\mathrm{T}}\boldsymbol{X}_i$$

is a solution of the linear system [9], and the constraints

$$\boldsymbol{\Omega}(\boldsymbol{Y}, H) + \boldsymbol{\Omega}(X^{\circ}, \boldsymbol{Y}^*)^{\mathrm{T}} = 2\,\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*)^{\mathrm{T}}\boldsymbol{x}$$
$$\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*) + \boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{\mathrm{T}} = 2\,\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*)^{\mathrm{T}}\boldsymbol{\Omega}(\boldsymbol{X}, \boldsymbol{Y}^*)$$

are admissible.

We remark that the above constraints have a simple geometric meaning when one considers the circular lattices in $\mathbb{E}^M$ as the stereographic projections of QLs in the Möbius sphere S^M; that is, as a special case of QLs subjected to quadratic constraints.

The symmetric lattice Given a QL $\boldsymbol{x}$ with rotation coefficients Q_{ij} and potentials ρ_i given by [11], then the functions $\tilde{Q}_{ij}$, defined by equation

$$\rho_j T_j \tilde{Q}_{ij} = \rho_i T_i Q_{ji}, \quad i \neq j$$

and called, because of their geometric interpretation, the backward rotation coefficients, satisfy the Darboux system [10] as well. A QL is called symmetric if its forward rotation coefficients Q_{ij} are also its backward rotation coefficients. Again the constraint is compatible with the geometric integrability scheme, that is, it propagates in the construction of the lattice. One can show that a QL is symmetric if and only if its rotation coefficients satisfy the following trilinear constraint:

$$(T_iQ_{ji})(T_jQ_{kj})(T_kQ_{ik}) = (T_jQ_{ij})(T_iQ_{ki})(T_kQ_{jk})$$
$$i, j, k \quad \text{distinct}$$

To obtain the corresponding reduction of the fundamental transformation we again need only half of the data. Given a solution $\boldsymbol{Y}_i^* : \mathbb{Z}^N \to \mathbb{V}^*$, of the linear system [8], then, because of the symmetric constraint, $\boldsymbol{Y}_i : \mathbb{Z}^N \to \mathbb{V}$, defined by

$$\boldsymbol{Y}_i = \rho_i (T_i \boldsymbol{Y}^*)^{\mathrm{T}}$$

is the solution of the linear system [9]; notice that, equivalently, we could start from $\boldsymbol{Y}_i$. The constraint

$$\boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*) = \boldsymbol{\Omega}(\boldsymbol{Y}, \boldsymbol{Y}^*)^{\mathrm{T}}$$

is then admissible and gives a new symmetric lattice.

There are other multidimensional reductions of the QL like, for example, the D-invariant and Egorov lattices or discrete versions of immersions of spaces of constant negative curvature. We remark that the transformations and reductions discussed above have also a clear interpretation on the level of the analytic methods.

Integrable Discrete Surfaces

In this section we present some distinguished examples of discrete integrable surfaces. Notice that, although the geometric integrability scheme is meaningless for $N = 2$, it can be applied indirectly, by considering the discrete surfaces, together with their transformations, as sublattices of multidimensional lattices.

We remark also that one can consider integrable evolutions of discrete curves, which give equations of the Ablowitz–Ladik hierarchy, and the corresponding integrable spin chains.

Discrete Isothermic Nets

An isothermic lattice is a two-dimensional circular lattice $\boldsymbol{x} : \mathbb{Z}^2 \to \mathbb{E}^M$ with harmonic quadrilaterals; that is, given $\boldsymbol{x}, T_1\boldsymbol{x}$ and $T_2\boldsymbol{x}$, then the point $T_1T_2\boldsymbol{x}$ is the intersection of the circle (passing through $\boldsymbol{x}, T_1\boldsymbol{x}$ and $T_2\boldsymbol{x}$) and the line passing through $\boldsymbol{x}$ and the meeting point of the tangents to the circle at $T_1\boldsymbol{x}$ and $T_2\boldsymbol{x}$ (see **Figure 5**). Therefore, given two discrete curves intersecting in the common vertex $\boldsymbol{x}_0$, the unique isothermic lattice can be found using the above "ruler and compass" construction.

Algebraically the reduction looks as follows. Any oriented plane in $\mathbb{E}^M$ can be identified with the complex plane $\mathbb{C}$. Given any four complex points z_1, z_2, z_3, and z_4, their complex cross-ratio is defined by

$$q(z_1, z_2, z_3, z_4) = \frac{(z_1 - z_2)(z_3 - z_4)}{(z_2 - z_3)(z_4 - z_1)}$$

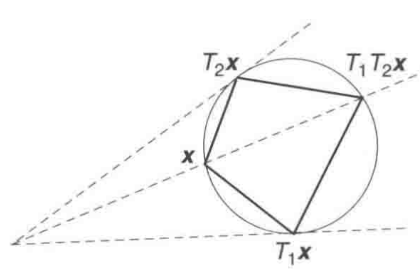


Figure 5 Elementary quadrilaterals of the isothermic lattice.

One can show that the cross-ratio is real if and only if the four points are cocircular or collinear. In particular, a harmonic quadrilateral with vertices numbered anticlockwise has cross-ratio equal to –1. Therefore, abusing the notation (it can be formalized using Clifford algebras), the isothermic lattice is defined by the condition

$$q(\boldsymbol{x}, T_1\boldsymbol{x}, T_1T_2\boldsymbol{x}, T_2\boldsymbol{x}) = -1$$

We remark that the definition of isothermic lattices can be slightly generalized allowing for the above cross-ratio to be a ratio of two real functions of single discrete variables.

The restriction of the Ribaucour transformation to the class of isothermic lattices, named after Darboux who constructed it for isothermic surfaces, has as its data a real parameter λ and the starting point $\mathcal{D}(\boldsymbol{x}_0)$, and can be described as follows. Given the elementary quadrilateral $\{\boldsymbol{x}, T_1\boldsymbol{x}, T_2\boldsymbol{x}, T_1T_2\boldsymbol{x}\}$ of the isothermic lattice, and given the point $\mathcal{D}(\boldsymbol{x})$, then the points $\mathcal{D}(T_1\boldsymbol{x})$ and $\mathcal{D}(T_2\boldsymbol{x})$ belong to the corresponding planes and are constructed from equations

$$q(\boldsymbol{x}, \mathcal{D}(\boldsymbol{x}), \mathcal{D}(T_1\boldsymbol{x}), T_1\boldsymbol{x}) = \lambda$$
$$q(\boldsymbol{x}, \mathcal{D}(\boldsymbol{x}), \mathcal{D}(T_2\boldsymbol{x}), T_2\boldsymbol{x}) = -\lambda$$

It turns out that the point $\mathcal{D}(T_1T_2\boldsymbol{x})$, constructed by the application of the geometric integrability scheme, is such that the quadrilateral $\{\mathcal{D}(\boldsymbol{x}), \mathcal{D}(T_1\boldsymbol{x}), \mathcal{D}(T_2\boldsymbol{x}), \mathcal{D}(T_1T_2\boldsymbol{x})\}$ is harmonic. Moreover, the construction of the Darboux transformation is compatible; that is, the new side quadrilaterals have the correct cross-ratios λ and $-\lambda$.

There are various integrable reductions of the isothermic lattice, for example, the constant mean curvature lattice and the minimal lattice.

Asymptotic Lattices and Their Reductions

An asymptotic lattice is a mapping $\boldsymbol{x}:\mathbb{Z}^2 \to \mathbb{R}^3$ such that any point $\boldsymbol{x}$ of the lattice is coplanar with its four nearest neighbors $T_1\boldsymbol{x}, T_2\boldsymbol{x}, T_1^{-1}\boldsymbol{x}, T_2^{-1}\boldsymbol{x}$ (see **Figure 6**). Such a plane is called the tangent plane of the asymptotic lattice in the point $\boldsymbol{x}$.

It can be shown that any asymptotic lattice $\boldsymbol{x}$ can be recovered from its suitably rescaled normal (to the tangent plane) field $\boldsymbol{N}:\mathbb{Z}^2 \to \mathbb{R}^3$ via the discrete analog of the Lelieuvre formulas

$$\Delta_1\boldsymbol{x} = (T_1\boldsymbol{N}) \times \boldsymbol{N}, \qquad \Delta_2\boldsymbol{x} = \boldsymbol{N} \times (T_2\boldsymbol{N}) \qquad [22]$$

By the compatibility of the Lelieuvre formulas, the normal field $\boldsymbol{N}$ satisfies the discrete Moutard equation

$$T_1T_2\boldsymbol{N} + \boldsymbol{N} = F(T_1\boldsymbol{N} + T_2\boldsymbol{N}) \qquad [23]$$

for some potential $F:\mathbb{Z}^2 \to \mathbb{R}$.

Given a scalar solution θ of the Moutard equation [23], a new solution $\mathcal{M}(\boldsymbol{N})$ of the Moutard equation, with the new potential

$$\mathcal{M}(F) = \frac{(T_1\theta)(T_2\theta)}{(T_1T_2\theta)\theta} F$$

can be found via the Moutard transformation equations

$$\mathcal{M}(T_1\boldsymbol{N}) \mp \boldsymbol{N} = \frac{\theta}{T_1\theta}(\mathcal{M}(\boldsymbol{N}) \mp T_1\boldsymbol{N}) \qquad [24]$$

$$\mathcal{M}(T_2\boldsymbol{N}) \pm \boldsymbol{N} = \frac{\theta}{T_2\theta}(\mathcal{M}(\boldsymbol{N}) \pm T_2\boldsymbol{N}) \qquad [25]$$

Now, via the Lelieuvre formulas [22], one can construct a new asymptotic lattice $\mathcal{M}(\boldsymbol{x}) = \boldsymbol{x} \pm \mathcal{M}(\boldsymbol{N}) \times \boldsymbol{N}$. The lines connecting corresponding points of the asymptotic lattices $\boldsymbol{x}$ and $\mathcal{M}(\boldsymbol{x})$ are tangent to both lattices. Such a $\mathbb{Z}^2$-family of lines in $\mathbb{R}^3$ is called Weingarten (or W for short) congruence. Notice that this is not a congruence as considered earlier.

Various integrable reductions of asymptotic lattices are known in the literature: pseudospherical lattices, asymptotic Bianchi lattices and isothermally asymptotic (or Fubini–Ragazzi) lattices, and discrete (proper and improper) affine spheres.

Formally, the Moutard transformation is a reduction of the (projective version of the) fundamental transformation for the Moutard reduction of the Laplace equation. However, the geometric relation between asymptotic lattices and QLs is more subtle and the geometric scenery of this connection is the line geometry of Plücker. Straight lines in $\mathbb{R}^3 \subset \mathbb{P}^3$ are considered there as points of the so-called Plücker quadric $\mathcal{Q}_P \subset \mathbb{P}^5$. A discrete asymptotic net in $\mathbb{P}^3$, viewed as the envelope of its tangent planes, corresponds to a congruence of isotropic lines in $\mathcal{Q}_P$, whose focal lattices represent the asymptotic directions. The discrete W-congruences are represented by two-dimensional QLs in the Plücker quadric.

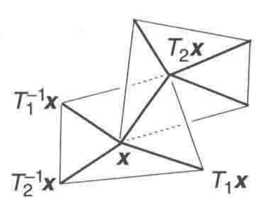


Figure 6 Asymptotic lattices.

The Koenigs Lattice

A two-dimensional QL $\boldsymbol{x}:\mathbb{Z}^2 \to \mathbb{P}^M$ is called a Koenigs lattice if, for every point $\boldsymbol{x}$ of the lattice,

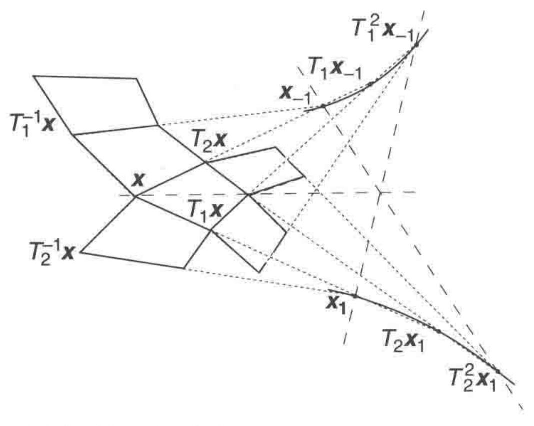


Figure 7 The Koenigs lattice.

the six points $x_{\pm 1}, T_i x_{\pm 1}, T_i^2 x_{\pm 1}, i=1,2$, of its Laplace transforms belong to a conic (see **Figure 7**). The nonlinear constraint in definition of the Koenigs lattice can be linearized, with the help of the Pascal "mystic hexagon" theorem, to the form that the line passing through x and T_1T_2x, the line passing through x_1 and $T_1^2x_{-1}$, and the line passing through x_{-1} and $T_2^2x_1$ intersect in a point.

Algebraically, the geometric Koenigs lattice condition means that the Laplace equation of the lattice in homogeneous coordinates $x:\mathbb{Z}^2 \to \mathbb{R}_*^{M+1}$ can be gauged into the form

$$T_1T_2x + x = T_1(Fx) + T_2(Fx) \qquad [26]$$

It turns out that, if N is a solution of the Moutard equation [23], then $x = T_1N + T_2N$ satisfies the Koenigs lattice equation. Therefore, the algebraic theory of the discrete Koenigs lattice equation [26], its (Koenigs) transformation, and the permutability of the superpositions of such transformations is based on the corresponding theory for the Moutard equation [23].

Geometrically, the Koenigs lattices are selected from the QLs as follows. Given a two-dimensional QL $x:\mathbb{Z}^2 \to \mathbb{P}^M$ and given a congruence $\mathfrak{l}$ with lines passing through the corresponding points of the lattice. Denote by $y_i = T_i^{-1}\mathfrak{l} \cap \mathfrak{l}, i=1,2$, points of the focal lattices of the congruence. For every line $\mathfrak{l}$, denote by $\imath$ the unique projective involution exchanging y_i with T_iy_i. If, for every congruence $\mathfrak{l}$, the lattice $\mathcal{K}(x):\mathbb{Z}^2 \to \mathbb{P}^M$, with points $\mathcal{K}(x) = \imath(x)$, is a QL, then the lattice x is a Koenigs lattice. The above construction gives also the corresponding reduction of the fundamental transformation.

A distinguished reduction of the Koenigs lattice is the quadrilateral Bianchi lattice. The natural continuous limit of the corresponding equation is equivalent to the Bianchi (or hyperbolic Ernst) system describing the interaction of planar gravitational waves.

Discrete Two-Dimensional Schrödinger Equation

In the previous sections we have discussed examples of integrable discrete geometries described by equations of hyperbolic type. Below we present some results associated with the elliptic case; it is remarkable that the QL provides a way to connect these two subjects.

Consider a solution $N:\mathbb{Z}^2 \to \mathbb{R}^3$ of the general self-adjoint five-point scheme on the star of the $\mathbb{Z}^2$ lattice

$$aT_1N + T_1^{-1}(aN) + bT_2N + T_2^{-1}(bN) - cN = 0 \qquad [27]$$

then the lattice $x:\mathbb{Z}^2 \to \mathbb{R}^3$ obtained by the Lelieuvre type formulas

$$\begin{aligned} \Delta_1 x &= -(T_2^{-1}b)N \times T_2^{-1}N \\ \Delta_2 x &= (T_1^{-1}a)N \times T_1^{-1}N \end{aligned} \qquad [28]$$

is a QL having N as normal (to the planes of elementary quadrilaterals) vector field.

The following gauge-equivalent form of eqn 27, namely

$$\begin{aligned} &\frac{\Gamma}{T_1\Gamma}T_1\psi + T_1^{-1}\left(\frac{\Gamma}{T_1\Gamma}\psi\right) + \frac{\Gamma}{T_2\Gamma}T_2\psi \\ &\quad + T_2^{-1}\left(\frac{\Gamma}{T_2\Gamma}\psi\right) - q\psi = 0 \end{aligned} \qquad [29]$$

an integrable discretization of the Schrödinger equation

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial x_2^2} - Q\psi = 0$$

is also the Lax operator associated with an integrable generalization of the Toda law to the square lattice.

The five-point scheme [27] is also a distinguished illustrative example of the sublattice theory. Indeed, it can be obtained restricting to the even sublattice $\mathbb{Z}_e^2$ the discrete Cauchy–Riemann equations

$$T_1T_2\phi - \phi = \mathrm{i}G(T_1\phi - T_2\phi) \qquad [30]$$

Because of the equivalence (on the discrete level!) between eqn [30] and the discrete Moutard equation [23], the five-point scheme [27] inherits integrability properties (Darboux-type transformations, superposition formulas, analytic methods of solution) from the corresponding (and simpler) integrability properties of the discrete Moutard equation.

See also: Bäcklund Transformations; $\bar{\partial}$-Approach to Integrable Systems; Integrable Discrete Systems; Integrable Systems and Algebraic Geometry; Integrable Systems and the Inverse Scattering Method; Integrable Systems: Overview; Nonlinear Schrödinger Equations; Sine-Gordon Equation; Stability Theory and KAM; Toda Lattices.

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Integrable Systems and Recursion Operators on Symplectic and Jacobi Manifolds

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Introduction

Let (M, ω) be a symplectic manifold of dimension $2n$. We denote by $\sharp$ the natural isomorphism between T^*M and TM, defined by the equation

$$i_{\sharp\alpha}\omega = -\alpha, \quad \alpha \in T^*M \qquad [1]$$

We say that $\sharp df$ is the Hamiltonian vector field defined by the Hamiltonian $f : M \to \mathbb{R}$.

Associated with the nondegenerated closed 2-form ω there is also a Poisson bracket on $C^\infty(M)$, the space of real differentiable functions on M, defined by

$$\{.,.\}_\omega : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$$
$$(f, g) \mapsto \{f, g\}_\omega = \omega(\sharp df, \sharp dg)$$

We say that two smooth functions $F, G : M \to \mathbb{R}$ are in involution if

$$\{F, G\}_\omega = 0 \qquad [2]$$

Suppose we have n independent smooth functions in involution $H_1, \ldots, H_n$, such that the associated Hamiltonian vector fields $X_1, \ldots, X_n$ are complete on the level manifold

$$M_a = \{x \in M : H_j(x) = a_j, j = 1, \ldots, n\} \qquad [3]$$

The classical theorem of Arnol'd–Liouville states that

1. the submanifold M_a is invariant with respect to each one of the Hamiltonian commuting flows generated by $H_1, \ldots, H_n$;
2. every connected component of M_a is diffeomorphic to a product of a Euclidean space by a torus, $\mathbb{R}^{n-k} \times \mathbb{T}^k$;
3. there exist coordinates $f_1, \ldots, f_{n-k}, \varphi_1, \ldots, \varphi_k$ in M_a such that the Hamiltonian systems in M_a, associated with the Hamiltonians H_j, have the form

$$\dot{f}_s = c_s^j \dot{\varphi}_m = \omega_m^j \quad (\omega \equiv \omega(a), c = \text{const.}) \qquad [4]$$

4. if M_a is compact then it is diffeomorphic to $\mathbb{T}^n$ and there exists a neighborhood of M_a on M, symplectically diffeomorphic to $\mathbb{B}^n \times \mathbb{T}^n$.

A completely integrable Hamiltonian system is a Hamiltonian vector field X, that admits n integrals $H_1, \ldots, H_n$ satisfying the hypothesis of Arnol'd–Liouville theorem.

It may happen that a system has more than n independent integrals of motion. In this case it is called superintegrable and not all the integrals are in involution. Supposing that

$$M_a = \{x \in M : H_j(x) = a_j, j = 1, \ldots, n+k\}$$

is compact and connected and that $H_1, \ldots, H_{n-k}$ commute with all the $n+k$ integrals, then M_a is diffeomorphic to the torus $\mathbb{T}^{n-k}$. In particular, if the system is maximally superintegrable, that is, $k = n-1, M_a$ is diffeomorphic to $T^1 = S^1$ and all the trajectories are closed.

To prove that a system is completely integrable, we have to find a sufficient number of integrals of the system in involution. The Lax pair is an extremely powerful tool in this task, although it does not guarantee the involution of the integrals found.

A Lax pair of a vector field X on a smooth manifold M is a pair of operators (L, M) such that

$$\dot{L} = [M, L] = ML - LM \qquad [5]$$

This equation is equivalent to

$$U^{-1}LU = L_0 \qquad [6]$$

where U is the solution operator of the Cauchy problem

$$\dot{U} = MU, \quad U(0) = I \qquad [7]$$

So, the eigenvalues of L are integrals of X. Notice that all the pairs $(L^k, M), k \in \mathbb{N}$, are Lax pairs of the system and we may conclude that the functions $\operatorname{tr} L^k, k \in \mathbb{N}$, are integrals of X.

The first goal of this article is to relate integrable Hamiltonian systems and recursion operators, where some of the most important properties of the latter are exhibited. Very naturally, the Poisson–Nijenhuis manifolds appear in this context and the Toda lattice is the example chosen in order to show the whole theory working in practice. Also, we see how recursion operators can help in the construction of quadratic algebras of integrals of motion and, in the last section, we present the generalization to Jacobi manifolds of the Nijenhuis structures defined for Poisson manifolds.

Integrable Systems on Poisson–Nijenhuis Manifolds

Let X be a vector field on a smooth manifold M. A recursion operator of X is a $(1,1)$-tensor R invariant of X:

$$\mathcal{L}_X R = 0 \qquad [8]$$

The $(1,1)$-tensors, and in particular the recursion operators, may be regarded as fiber endomorphisms of TM. So, given a $(1,1)$-tensor R, we denote by ${}^tR : T^*M \to T^*M$ the transpose of $R : TM \to TM$, that is,

$$\langle {}^tR(\alpha), X\rangle = \langle \alpha, R(X)\rangle, \quad \alpha \in T^*M,\ X \in TM \qquad [9]$$

where $\langle .,. \rangle$ denotes the canonical pairing between T^*M and TM.

Recursion operators also generate symmetries. If R is a recursion operator and Y is a symmetry of X, that is, $[X, Y] = 0$, then RY is also a symmetry of X. So, given a recursion operator R of X, we may construct a sequence of symmetries of X, $R^k Y, k \in \mathbb{N}$.

The Nijenhuis torsion of a $(1,1)$-tensor R is the $(1,2)$-tensor $\mathcal{T}(R)$ defined by

$$\begin{aligned}\mathcal{T}(R)(X, Y) = [RX, RY] - R([X, RY] + [RX, Y] \\ -R[X, Y]), \quad X, Y \in \mathfrak{X}(M)\end{aligned} \qquad [10]$$

A Nijenhuis operator is a $(1,1)$-tensor, R, with vanishing Nijenhuis torsion, that is,

$$\mathcal{L}_{RX} R = R\mathcal{L}_X R \qquad [11]$$

These operators can generate sequences of closed 1-forms. If R is a Nijenhuis operator and α is a closed 1-form such that $\mathrm{d}{}^tR(\alpha) = 0$, then $\mathrm{d}{}^tR^k(\alpha) = 0, k \in \mathbb{N}$. In the particular case of α being exact, that is, $\alpha = \mathrm{d}f$ and the first cohomology group being trivial, then we have a sequence of local integrals of motion $\mathrm{d}f_k = {}^tR^k(\mathrm{d}f)$.

A Nijenhuis recursion operator R and a symmetry Y of a vector field X lead to a sequence of commuting symmetries $R^k Y, k \in \mathbb{N}$,

$$[R^i Y, R^j Y] = 0, \quad i, j \in \mathbb{N} \qquad [12]$$

To define the integrability in terms of a $(1,1)$-tensor is of special relevance when we try to extend everything to the infinite-dimensional case.

Notice that in coordinates $(q_1, \ldots, q_n)$, the condition [8] is equivalent to

$$\dot{R} = [A, R] \qquad [13]$$

where A is the $n \times n$ matrix defined by

$$A_{ij} = \left[\frac{\partial X^i}{\partial q_j}\right]$$

and $X^j = X(q_j) = \dot{q}_j, j = 1, \ldots, n$. So, the pair (R, A) is a local Lax pair of the system and the eigenvalues of R are integrals of X.

If a recursion operator R of a vector field X on a manifold M has vanishing Nijenhuis torsion and n doubly degenerated eigenvalues λ_i, with nowhere-vanishing differentials, $(d\lambda_i)_p \neq 0$, then X defines a completely integrable Hamiltonian system.

Now suppose X defines a completely integrable Hamiltonian system with Hamiltonian H on a symplectic manifold (M, ω). Let $(I_1, \ldots, I_n, \varphi_1, \ldots, \varphi_n)$ be the action-angle variables in a neighborhood of an invariant torus. Two cases may happen:

1. The Hamiltonian H is separable in the action variable, that is,

$$H = \sum_k H_k(I_k) \qquad [14]$$

In this case, the $(1,1)$-tensor

$$R = \sum_k \lambda_k(I_k)\left(dI_k \otimes \frac{\partial}{\partial I_k} + d\varphi_k \otimes \frac{\partial}{\partial \varphi_k}\right) \qquad [15]$$

where λ_k are functions with nowhere-vanishing differentials, is a recursion operator of X, and has vanishing Nijenhuis torsion and doubly degenerated eigenvalues.

2. The Hamiltonian has nonvanishing Hessian

$$\det\left(\frac{\partial^2 H}{\partial I_k \partial I_j}\right) \neq 0 \qquad [16]$$

In this case we may define new coordinates

$$\nu_k = \frac{\partial H}{\partial I_k}, \quad k = 1, \ldots, n \qquad [17]$$

and a new symplectic structure

$$\omega_1 = \sum_k d\nu_k \wedge d\varphi_k = \sum_{k,j} \frac{\partial^2 H}{\partial I_k \partial I_j} dI_k \wedge d\varphi_j \qquad [18]$$

The vector field X is Hamiltonian with respect to ω_1, with Hamiltonian

$$H = \frac{1}{2}\sum_k \nu_k^2 \qquad [19]$$

and the $(1,1)$-tensor

$$R = \sum_k \lambda_k(I_k)\left(d\nu_k \otimes \frac{\partial}{\partial \nu_k} + d\varphi_k \otimes \frac{\partial}{\partial \varphi_k}\right) \qquad [20]$$

is a recursion operator of X.

Nijenhuis operators also allow the construction of master symmetries from conformal ones.

A conformal symmetry of a tensor field T is a vector field Z such that

$$\mathcal{L}_Z T = \lambda T, \quad \text{for some constant } \lambda$$

A master symmetry of a vector field X is a vector field Y such that

$$[X, [X, Y]] = 0, \quad \text{but } [X, Y] \neq 0$$

Let R be a recursion operator of X_0 and Z_0 be a conformal symmetry of X_0 and R such that

$$\mathcal{L}_{Z_0} X_0 = \lambda X_0 \quad \text{and} \quad \mathcal{L}_{Z_0} R = R \qquad [21]$$

for some constants λ, μ.

If R is also a Nijenhuis operator, then defining the sequences of commuting symmetries $X_k = R^k X_0$ and of conformal symmetries $Z_k = R^k Z_0, k \in \mathbb{N}$, we have, for all $k, j \in \mathbb{N}_0$,

$$\mathcal{L}_{Z_k} R = \mu R^{k+1} \qquad [22]$$

$$[Z_k, Z_j] = \mu(j - k) Z_{j+k} \qquad [23]$$

$$[Z_k, X_j] = (\lambda + j\mu) X_{k+j} \qquad [24]$$

A bi-Hamiltonian manifold is a smooth manifold M endowed with two linearly independent Poisson tensors Λ_0, Λ_1, compatible in the sense that their Schouten bracket vanishes, $[\Lambda_0, \Lambda_1] = 0$.

A vector field is said to be bi-Hamiltonian if it is Hamiltonian with respect to both Poisson structures. The equation that rules the flow of this vector field is said to be a bi-Hamiltonian system.

When one of the Poisson structures is obtained from the other by means of a Nijenhuis operator, we obtain a Poisson–Nijenhuis manifold. Hence, a Poisson–Nijenhuis manifold is a differentiable manifold M endowed with a Poisson tensor Λ and a $(1,1)$-tensor R such that

$$R\Lambda^\sharp = \Lambda^{\sharp t} R, \quad [R\Lambda, \Lambda] = 0 \text{ and } [R\Lambda, R\Lambda] = 0$$

A classical example is the one of a bi-Hamiltonian manifold $(M, \Lambda_0, \Lambda_1)$ where Λ_0 is nondegenerated. In this case we may define the Nijenhuis operator $R = \Lambda_1^\sharp \Lambda_0^{\sharp -1}$ and the manifold M is a Poisson–Nijenhuis one.

The characteristics of the Poisson–Nijenhuis manifold guarantee that all the bivectors $\Lambda_k = R^k \Lambda$ are compatible Poisson tensors and the manifold is not just bi-Hamiltonian but multi-Hamiltonian.

From what we saw, a Hamiltonian system is completely integrable if and only if it is bi-Hamiltonian

in a neighborhood of an invariant torus with the eigenvalues of the existing recursion operator providing its complete integrability. These Poisson–Nijenhuis manifolds appear quite frequently in dynamics and allow us to obtain some interesting properties easily. We finish this section with the Toda lattice. This system is a good illustration of what has been said until now.

Consider $\mathbb{R}^{2n-1}$ with coordinates $(a_1, \ldots, a_{n-1}, b_1, \ldots, b_n)$ equipped with the following compatible Poisson tensors:

$$\Lambda_0 = \frac{1}{4}\sum_{i=1}^{n-1} a_i \frac{\partial}{\partial a_i} \wedge \left(\frac{\partial}{\partial b_i} - \frac{\partial}{\partial b_{i+1}}\right) \qquad [25]$$

$$\Lambda_1 = \sum_{i=1}^{n-1} a_i^2 \frac{\partial}{\partial b_{i+1}} \wedge \frac{\partial}{\partial b_i} - \frac{1}{4}\sum_{i=1}^{n-1} a_i \frac{\partial}{\partial a_i} \wedge \left(a_{i+1}\frac{\partial}{\partial a_{i+1}} + 2b_{i+1}\frac{\partial}{\partial b_{i+1}} - 2b_i\frac{\partial}{\partial b_i}\right) \qquad [26]$$

Not only these two Poisson tensors are degenerated but also there is no Nijenhuis operator that transforms Λ_0 into Λ_1. This can be seen considering the 1-form $\sum_{i=1}^{n} db_i$. This 1-form belongs to the kernel of Λ_0 but not to the kernel of Λ_1. So, the bi-Hamiltonian manifold $(\mathbb{R}^{2n-1}, \Lambda_0, \Lambda_1)$ is not a Poisson–Nijenhuis one.

The Toda lattice is the bi-Hamiltonian system in $\mathbb{R}^{2n-1}$:

$$X_1 = \Lambda_0^\sharp(dH_1) = \Lambda_1^\sharp(dH_0) \qquad [27]$$

defined by the Hamiltonians

$$H_0 = 2\sum_{i=1}^{n} b_i, \qquad H_1 = 4\sum_{i=1}^{n-1} a_i^2 + 2\sum_{i=1}^{n} b_i^2 \qquad [28]$$

that is,

$$\begin{aligned} \dot a_i &= a_i(b_{i+1} - b_i), \quad \text{if } 1 \le i \le n-1 \\ \dot b_1 &= 2a_1^2 \\ \dot b_i &= 2(a_i^2 - a_{i-1}^2), \quad \text{if } 2 \le i \le n-1 \\ \dot b_n &= -2a_{n-1}^2 \end{aligned}$$

Since we do not have a Nijenhuis operator in this setting, we are going to consider a new system in $\mathbb{R}^{2n}$ that reduces to the Toda lattice, derive a hierarchy of Hamiltonians, symmetries, Poisson tensors, conformal symmetries and the associated relations and then transport everything to $\mathbb{R}^{2n-1}$ by reduction.

Consider the Flaschka transformation

$$\pi : \mathbb{R}^{2n} \to \mathbb{R}^{2n-1}$$
$$(q_1, \ldots, q_n, p_1, \ldots, p_n) \mapsto (a_1, \ldots, a_{n-1}, b_1, \ldots, b_n)$$

where

$$a_i = \frac{1}{2}\exp\left(\frac{q_i - q_{i+1}}{2}\right), \qquad b_j = -\frac{1}{2}p_j$$
$$i = 1, \ldots, n-1, \quad j = 1, \ldots, n \qquad [29]$$

This application is a Poisson morphism between $(\mathbb{R}^{2n}, \widetilde{\Lambda}_0, \widetilde{\Lambda}_1)$ and $(\mathbb{R}^{2n-1}, \Lambda_0, \Lambda_1)$, where

$$\widetilde{\Lambda}_0 = \sum_{i=1}^{n} \frac{\partial}{\partial p_i} \wedge \frac{\partial}{\partial q_i} \qquad [30]$$

$$\widetilde{\Lambda}_1 = \sum_{i=1}^{n-1} e^{q_i - q_{i+1}} \frac{\partial}{\partial p_{i+1}} \wedge \frac{\partial}{\partial p_i} + \sum_{i=1}^{n}\left(p_i \frac{\partial}{\partial q_i} \wedge \frac{\partial}{\partial p_i} + \sum_{i<j} \frac{\partial}{\partial q_j} \wedge \frac{\partial}{\partial q_i}\right) \qquad [31]$$

The Poisson tensor $\widetilde{\Lambda}_0$ is nondegenerated and we may define the Nijenhuis operator $R = \widetilde{\Lambda}_1^\sharp \widetilde{\Lambda}_0^{\sharp -1}$. So, $(\mathbb{R}^{2n}, \widetilde{\Lambda}_0, \widetilde{\Lambda}_1)$ is a Poisson–Nijenhuis manifold and the bivectors of the sequence $(\widetilde{\Lambda}_k = R^k \widetilde{\Lambda}_0), k \in \mathbb{N}$, are compatible Poisson tensors.

The Toda lattice is the reduced bi-Hamiltonian system, by means of the Flaschka transformation, of the bi-Hamiltonian system

$$\widetilde{X}_1 = \widetilde{\Lambda}_0^\sharp(d\widetilde{H}_1) = \widetilde{\Lambda}_1^\sharp(d\widetilde{H}_0) \qquad [32]$$

where

$$\widetilde{H}_0 = \sum_{i=1}^{n} p_i, \qquad \widetilde{H}_1 = \sum_{i=1}^{n} \frac{p_i^2}{2} + \sum_{i=1}^{n-1} e^{q_i - q_{i+1}} \qquad [33]$$

We may define the sequence of commuting vector fields $\widetilde{X}_k = R^{n-1}\widetilde{X}_1, k \in \mathbb{N}$, and the sequence of Hamiltonians $d\widetilde{H}_k = {}^tR^k(d\widetilde{H}_0), k \in \mathbb{N}$, first integrals of all the vector fields $\widetilde{X}_j$ and in involution with respect to all the Poisson structures $\widetilde{\Lambda}_j$.

Moreover, considering the conformal symmetry of $\widetilde{\Lambda}_0, \widetilde{\Lambda}_1$, and $\widetilde{H}_0$ defined by

$$\widetilde{Z}_0 = \sum_{i=1}^{n} (n+1-2i)\frac{\partial}{\partial q_i} + \sum_{i=1}^{n} p_i \frac{\partial}{\partial p_i} \qquad [34]$$

we have the following relations on $\mathbb{R}^{2n}$:

$$\mathcal{L}_{\widetilde{Z}_m} R = R^{m+1} \qquad [35]$$

$$[\widetilde{Z}_m, \widetilde{Z}_k] = (k - m)\widetilde{Z}_{k+m} \quad [36]$$

$$[\widetilde{Z}_k, \widetilde{X}_{m+1}] = m\widetilde{X}_{k+m+1} \quad [37]$$

$$\mathcal{L}_{\widetilde{Z}_k}\widetilde{\Lambda}_m = (m - k - 1)\widetilde{\Lambda}_{k+m} \quad [38]$$

$$\widetilde{Z}_k.\widetilde{H}_m = (m + n + 1)\widetilde{H}_{k+m} \quad [39]$$

Although we do not have a Nijenhuis operator on $(\mathbb{R}^{2n-1}, \Lambda_0, \Lambda_1)$, the deformation relations [35]–[39], obtained for the Poisson–Nijenhuis manifold $(\mathbb{R}^{2n}, \widetilde{\Lambda}_0, \widetilde{\Lambda}_1)$, may be reduced to the bi-Hamiltonian manifold $(\mathbb{R}^{2n-1}, \Lambda_0, \Lambda_1)$ by means of the Flaschka transformation π.

Recursion Operators and Algebras of Integrals of Motion

A master integral of a vector field X is a differentiable function g such that

$$\mathcal{L}_X\mathcal{L}_X g = 0 \quad \text{and} \quad \mathcal{L}_X g \neq 0 \quad [40]$$

So, a master integral g generates an integral of motion $\mathcal{L}_X g$ of the system X. It is worth noticing that if f and g are master integrals, then not only $\mathcal{L}_X f$ and $\mathcal{L}_X g$ are integrals but also $(\mathcal{L}_X f)g - f(\mathcal{L}_X g)$ is an integral of the system. This means that several master integrals may lead to extra integrals of motion. This procedure often leads to the construction of the integrals which provide the superintegrability of the system in consideration. This is the case of, for instance, the generalized rational Calogero–Moser system or the geodesic flow on the sphere.

Recursion operators are often used to construct sequences of master symmetries of vector fields. The obvious connection between master symmetries and master integrals carries the recursion operators to this level. In many cases, the integrals of motion generated by the master integrals constructed on the basis of the existence of a recursion operator close in a quadratic algebra with respect to the Poisson structure we are considering (by quadratic algebra we mean that the brackets between the generators are polynomials of degree 2 in the generators).

Let X be a vector field on a manifold M, R a Nijenhuis operator which is also a recursion operator of X, and P a $(1,1)$-tensor such that

$$\mathcal{L}_X P = a(R)$$

and

$$\mathcal{L}_{PX} R = b(R)$$

where a and b are polynomials with constant coefficients. The sequences $X_i = R^i X$, $Y_i = R^i(PX)$, $i \in \mathbb{N}_0$, $X_{-1} = Y_{-1} = 0$ satisfy

$$[X_i, X_j] = 0 \quad [41]$$

$$[X_i, Y_j] = a(R)X_{i+j} - ib(R)X_{i+j-1} \quad [42]$$

$$[Y_i, Y_j] = (j - i)b(R)Y_{i+j-1} \quad [43]$$

If (M, Λ) is a nondegenerated Poisson manifold with trivial first cohomology group, $R\Lambda$ is a bivector and X and Y are Hamiltonian vector fields with respect to Λ and $R\Lambda$, that is, there exist functions H_0, H_1, G_0, and G_1 satisfying

$$X = \Lambda^\sharp(dH_1) = R\Lambda^\sharp(dH_0)$$
$$Y = \Lambda^\sharp(dG_1) = R\Lambda^\sharp(dG_0)$$

then the sequences of exact differentials

$$^tR^i(dH_1) = dH_i \quad \text{and} \quad ^tR^i(dG_1) = dG_i$$

may be constructed. In this case, the functions G_j are master integrals of all the vector fields X_i and the integrals $X_i(G_j)$ and $L^i_{k,j} = X_i(G_k)G_j - X_i(G_j)G_k$, $j, k \in \mathbb{N}_0$, close in a quadratic algebra with respect to the Poisson bracket associated with Λ.

If M is not a Poisson manifold but we can find a master integral G of all the vector fields X_i of the sequence, then the functions $G_j = Y_j(G)$ are also master integrals of the same vector fields and the functions $X_i(G_j)$ and $L^i_{k,j} = X_i(G_k)G_j - X_i(G_j)G_k$ are integrals of X_i.

Now let us consider the completely integrable bi-Hamiltonian system case. In a neighborhood of an invariant torus, a completely integrable bi-Hamiltonian system may be written in the form

$$\widetilde{H}(y_1, \ldots, y_n) = y_1 + \cdots + y_n \quad [44]$$

with

$$\Lambda_0 = \sum_{i=1}^n \frac{\partial}{\partial y_i} \wedge \frac{\partial}{\partial \phi_i}$$
$$\Lambda_1 = \sum_{i=1}^n y_i \frac{\partial}{\partial y_i} \wedge \frac{\partial}{\partial \phi_i}$$

the compatible Poisson tensors that provide the complete integrability of the bi-Hamiltonian system. In this case, we may define the recursion operator

$$R = \sum_{i=1}^n y_i \left(\frac{\partial}{\partial y_i} \otimes dy_i + \frac{\partial}{\partial \phi_i} \otimes d\phi_i \right)$$

for which $\Lambda_1 = R\Lambda_0$, and the bi-Hamiltonian vector field

$$X = \Lambda_0^\sharp(d\widetilde{H}) = \Lambda_1^\sharp\left[d\left(\sum_{i=1}^{n}\ln(y_i)\right)\right]$$

The (1, 1)-tensor

$$P = \sum_{i=1}^{n}\left(\phi_i\frac{\partial}{\partial\phi_i}\otimes d\phi_i + \frac{\partial}{\partial y_i}\otimes dy_i\right)$$

satisfies $\mathcal{L}_X P = \mathrm{Id}$ and $\mathcal{L}_{PX}R = 0$. So, the vector fields

$$Y_k = R^k(PX) = \sum_{i=1}^{n} y_i^k\phi_i\frac{\partial}{\partial\phi_i}$$

and the function $G = \sum_{i=1}^{n} y_i\phi_i$ help defining the functions $G_i = Y_i(G), i\in\mathbb{N}_0$.

The integrals of X_k

$$X_k(G_j) \quad\text{and}\quad L_{i,j}^k = X_k(G_i)G_j - G_iX_k(G_j) \qquad [45]$$

happen to close in a quadratic algebra with respect to the bracket defined by Λ_0.

Recursion Operators on Jacobi Manifolds

In this section we extend the notion of Poisson–Nijenhuis manifold to the Jacobi setting.

Let M be a smooth manifold with a bivector field Λ and a vector field E. We equip the space $C^\infty(M)$ with the bracket

$$\{f,g\} = \Lambda(df,dg) + fE(g) - gE(f)$$

which is bilinear and skew-symmetric, and satisfies the Jacobi identity if and only if

$$[\Lambda,\Lambda] = -2E\wedge\Lambda \quad\text{and}\quad [E,\Lambda] = 0 \qquad [46]$$

When these conditions are satisfied, (M,Λ,E) is called a Jacobi manifold with Jacobi bracket $\{\cdot,\cdot\}$. The pair $(C^\infty(M),\{,\})$ is a local Lie algebra in the sense of Kirillov. If the vector field E identically vanishes on M, eqns [46] reduce to $[\Lambda,\Lambda]=0$ and (M,Λ) is just a Poisson manifold. But there are other examples of Jacobi manifolds that are not Poisson, for example, contact manifolds.

We denote by $(\Lambda,E)^\#: T^*M\times\mathbb{R}\to TM\times\mathbb{R}$ the vector bundle map associated with (Λ,E), that is, for all α,β sections of T^*M and $f\in C^\infty(M)$,

$$(\Lambda,E)^\#(\alpha,f) = (\Lambda^\#(\alpha) + fE, -i_E\alpha)$$

Let $\mathcal{R}:\mathfrak{X}(M)\times C^\infty(M)\to\mathfrak{X}(M)\times C^\infty(M)$ be a $C^\infty(M)$-linear map defined by

$$\mathcal{R}(X,f) = (NX + fY, i_X\gamma + gf) \qquad [47]$$

where N is a tensor field of type $(1,1)$ on M, $Y\in\mathfrak{X}(M)$, $\gamma\in\Omega^1(M)$ and $g\in C^\infty(M)$. Let us denote by $\mathcal{T}(\mathcal{R})$ the Nijenhuis torsion of $\mathcal{R}$ with respect to the Lie bracket on $\mathfrak{X}(M)\times C^\infty(M)$ given by

$$[(X,f),(Z,h)] = ([X,Z], X(h) - Z(f)) \qquad [48]$$

As in the case of Poisson manifolds, if $\mathcal{R}$ has a vanishing Nijenhuis torsion, we call $\mathcal{R}$ a Nijenhuis operator.

Suppose now that M is equipped with a Jacobi structure (Λ_0,E_0) and a Nijenhuis operator $\mathcal{R}$. Then, we may define a bivector field Λ_1 and a vector field E_1 on M, by setting

$$(\Lambda_1,E_1)^\# = \mathcal{R}\circ(\Lambda_0,E_0)^\#$$

If one looks for the conditions that imply that the pair (Λ_1,E_1) defines a new Jacobi structure on M compatible with (Λ_0,E_0), in the sense that $(\Lambda_0+\Lambda_1,E_0+E_1)$ is again a Jacobi structure, one finds that Λ_1 is skew-symmetric if and only if $\mathcal{R}\circ(\Lambda_0,E_0)^\# = (\Lambda_0,E_0)^\#\circ{}^t\mathcal{R}$. When Λ_1 is skew-symmetric, (Λ_1,E_1) defines a Jacobi structure on M if and only if, for all $(\alpha,f),(\beta,h)\in\Omega^1(M)\times C^\infty(M)$,

$$\mathcal{T}(\mathcal{R})\Big((\Lambda_0,E_0)^\#(\alpha,f),(\Lambda_0,E_0)^\#(\beta,h)\Big) = \mathcal{R}\circ(\Lambda_0,E_0)^\#(\mathcal{C}((\Lambda_0,E_0),\mathcal{R})((\alpha,f),(\beta,h)))$$

where $\mathcal{C}((\Lambda_0,E_0),\mathcal{R})$ is the Magri concomitant of (Λ_0,E_0) and $\mathcal{R}$. In the case where (Λ_1,E_1) is a Jacobi structure, it is compatible with (Λ_0,E_0) if and only if, for all $(\alpha,f),(\beta,h)\in\Omega^1(M)\times C^\infty(M)$,

$$(\Lambda_0,E_0)^\#(\mathcal{C}((\Lambda_0,E_0),\mathcal{R})((\alpha,f),(\beta,h))) = 0$$

A Jacobi–Nijenhuis manifold $(M,(\Lambda_0,E_0),\mathcal{R})$ is a Jacobi manifold (M,Λ_0,E_0) with a Nijenhuis operator $\mathcal{R}$ such that: (1) $\mathcal{R}\circ(\Lambda_0,E_0)^\# = (\Lambda_0,E_0)^\#\circ{}^t\mathcal{R}$ and (2) the map $(\Lambda_0,E_0)^\#\circ\mathcal{C}((\Lambda_0,E_0),\mathcal{R})$ identically vanishes. $\mathcal{R}$ is called the recursion operator of $(M,(\Lambda_0,E_0),\mathcal{R})$.

A recursion operator on a Jacobi–Nijenhuis manifold displays a hierarchy of Jacobi–Nijenhuis structures on the manifold. In fact, if $((\Lambda_0,E_0),\mathcal{R})$ is a Jacobi–Nijenhuis structure on M, there exists a hierarchy $((\Lambda_k,E_k),k\in\mathbb{N})$ of Jacobi structures on M, which are pairwise compatible. For all $k\in\mathbb{N}$, (Λ_k,E_k) is the Jacobi structure associated with the vector bundle map $(\Lambda_k,E_k)^\#$ given by $(\Lambda_k,E_k)^\# = \mathcal{R}^k\circ(\Lambda_0,E_0)^\#$. Moreover, for all $k,l\in\mathbb{N}$, the pair $((\Lambda_k,E_k),\mathcal{R}^l)$ defines a Jacobi–Nijenhuis structure on M.

See also: Bi-Hamiltonian Methods in Soliton Theory; Classical *r*-Matrices, Lie Bialgebras, and Poisson Lie Groups; Contact Manifolds; Integrable Systems and Algebraic Geometry; Integrable Systems: Overview;

Multi-Hamiltonian Systems; Recursion Operators in Classical Mechanics.

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Integrable Systems and the Inverse Scattering Method

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Introduction

A British experimentalist, J S Russell, first observed a soliton in 1834 while riding on horseback beside a narrow barge channel. He challenged the theoreticians of the day "to predict the discovery after it happened, that is to give an *a priori* demonstration *a posterori*." This work created a controversy which, in fact, lasted almost 50 years, and which involved such distinguished scientists as Stokes and Airy. It was resolved by Korteweg and deVries in 1895, who derived the KdV equation as an approximation to water waves,

$$\frac{\partial q}{\partial t} + 6q\frac{\partial q}{\partial x} + \frac{\partial^3 q}{\partial x^3} = 0 \qquad [1]$$

This equation is a nonlinear partial differential equation (PDE) of the evolution type, where t and x are related to time and space respectively, and $q(x,t)$ is related to the height of the wave above the mean water level. Korteweg and de Vries were able to show that equation [1] supports a particular solution that exhibits the behavior described by Russell. This solution, which was later called 1-soliton solution, is given by

$$q_1(x - p^2 t) = \frac{p^2/2}{\cosh^2((1/2)p(x - p^2 t) + c)} \qquad [2]$$

where p, c are constants. The location of this soliton at time t, that is, its maximum position, is given by $p^2 - 2c/p$, its velocity is given by p^2, and its amplitude by $p^2/2$. Thus, faster solitons are higher and narrower. It should be noted that q_1 is a traveling-wave solution, that is, q_1 depends only on the variable $X = x - p^2 t$, thus in this case the PDE [1] reduces (after integration) to the second-order ordinary differential equation (ODE)

$$-p^2 q_1(X) + 3q_1^2(X) + \frac{d^2 q_1}{dX^2}(X) = 0$$

Under the assumption that q and dq/dX tend to zero as $|X| \to \infty$, this ODE yields the 1-soliton solution [2].

The problem of finding a solution describing the interaction of two 1-soliton solutions is much more difficult and was not addressed by Korteweg and deVries. This question was studied by M Kruskal and N Zabusky in 1965. Studying numerically the interaction of two solutions of the form [2] (i.e., two solutions corresponding to two different p_1 and p_2), Kruskal and Zabusky discovered the defining property of solitons: after interaction, these waves regained exactly the shapes they had before. This posed a new challenge to mathematicians, namely to explain analytically the interaction properties of such coherent waves. In order to resolve this challenge one needs to develop a larger class of solutions than the 1-soliton solution. We note that eqn [1] is nonlinear and no effective method to solve such nonlinear equations existed at that time.

Gardner *et al.* (1967) not only derived an explicit solution describing the interaction of an arbitrary number of solitons, but also discovered what was to

evolve into a new method of mathematical physics. The 2-soliton solution is given by

$$q_2(x,t) = \frac{2(p_1^2 e^{\eta_1} + p_2^2 e^{\eta_2}) + 4e^{\eta_1+\eta_2}(p_1 - p_2)^2 + 2A_{12}(p_2^2 e^{2\eta_1+\eta_2} + p_1^2 e^{\eta_1+2\eta_2})}{(1 + e^{\eta_1} + e^{\eta_2} + A_{12}e^{\eta_1+\eta_2})^2} \qquad [3]$$

where

$$\eta_j = p_j x - p_j^3 t + \eta_j^0, j = 1, 2, \qquad A_{12} = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2}$$

and p_j, η_j^0 are constants. A snapshot of this solution with $p_1 = 1, p_2 = 2$ is given in **Figure 1**. After some time the taller soliton will overtake the shorter one and the only effect of the interaction will be a "phase shift," that is, a change in the position the two solitons would have reached without interaction.

Regarding the general method introduced in Gardner *et al.* (1967), we note that if eqn [1] is formulated on the infinite line, then the most interesting problem is the solution of the initial-value problem: given initial data $q(x,0) = q_0(x)$ which decay as $|x| \to \infty$, find $q(x,t)$. If q_0 is small and qq_x can be neglected, then eqn [1] becomes linear and $q(x,t)$ can be found using the Fourier transform,

$$q(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx+ik^3t}\hat{q}_0(k)\,dk \qquad [4a]$$

where

$$\hat{q}_0(k) = \int_{-\infty}^{\infty} e^{-ikx}q_0(x)\,dx \qquad [4b]$$

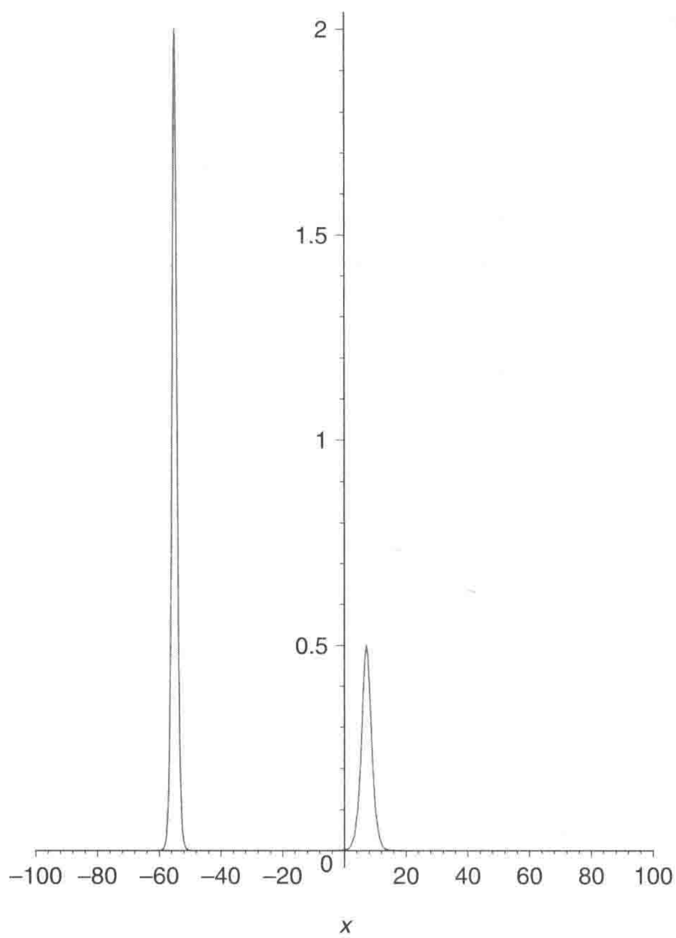


Figure 1 A snapshot of the 2-soliton solution of the KdV equation.

The remarkable discovery of Gardner *et al.* (1967) is that for eqn [1] there exists a "nonlinear analog" of the Fourier transform capable of solving the initial-value problem even if q_0 is not small. Although this nonlinear Fourier transform cannot in general be written in closed form, $q(x,t)$ can be expressed through the solution of a linear integral equation, or more precisely through the solution of a linear 2×2 matrix Riemann–Hilbert (RH) problem (see the section "A nonlinear Fourier transform"). This linear integral equation is uniquely specified in terms of $q_0(x)$. For particular initial data, $q(x,t)$ can be written explicitly. For example, if $q_0(x) = q_1(x)$, where $q_1(x)$ is obtained by evaluating eqn [2] at $t = 0$, then $q(x,t) = q_1(x - p^2 t)$. Similarly, if $q_0(x) = q_2(x,0)$, where $q_2(x,0)$ is obtained by evaluating eqn [3] at $t = 0$, then $q(x,t) = q_2(x,t)$.

The most important question, both physically and mathematically, is the description of the long-time behavior of the solution of the initial-value problem mentioned above. If the nonlinear term of eqn [1] can be neglected, one finds a linear dispersive equation. In this case different waves travel with different wave speeds, these waves cancel each other out and the solution decays to zero as $t \to \infty$. Indeed, using the stationary-phase method to compute the large t behavior of the integral appearing in eqn [4a], it can be shown that $q(x,t)$ decays like $0(1/\sqrt{t})$ as $t \to \infty$, $x/t = 0(1)$. The situation with the KdV equation is more interesting: dispersion is balanced by nonlinearity and $q(x,t)$ has a "nontrivial" asymptotic behavior as $t \to \infty$. Indeed, using a nonlinear analog of the steepest descent method discovered by Deift and Zhou (1993) to analyze the RH problem mentioned earlier, it can be shown that $q(x,t)$ asymptotes to $q_N(x,t)$, where $q_N(x,t)$ is the exact N-soliton solution. This underlines the physical and mathematical significance of solitons: they are the coherent structures emerging from any initial data as $t \to \infty$. This implies that if a nonlinear phenomenon is modeled by the KdV equation on the infinite line, then one can immediately predict the structure of the solution as $t \to \infty$, $x/t = 0(1)$: it will consist of N ordered single solitons, where the highest soliton occurs to the right; the number N and the parameters p_j and η_j^0 depend on the particular initial data $q_0(x)$. It should

be noted that this result can be obtained only using the machinery of the theory of integrability, and until now cannot be obtained using standard PDE techniques.

So far we have concentrated on the KdV equation. However, there exist numerous other equations which exhibit similar behavior. Such equations are called "integrable" and the method of solving their initial-value problem is called the "inverse-scattering" or "inverse-spectral" method.

The following section presents a brief historical review of some of the important developments of soliton theory. Next, typical solitons, lumps, and dromions are given. The inverse-spectral method is discussed in the penultimate section. Finally, the extension of this method to boundary-value problems is briefly discussed.

Important Analytical Developments in Soliton Theory

Lax (1968) introduced the so-called Lax pair formulation of the KdV. In an example, he showed that eqn [1] can be written as the compatibility condition of the following pair of linear eigenvalue equations for the eigenfunction $\psi(x,t,k)$:

$$\psi_{xx} + (q + k^2)\psi = 0 \qquad [5a]$$

$$\psi_t + (2q - 4k^2)\psi_x - (q_x + \nu)\psi = 0, \quad k \in \mathbb{C} \qquad [5b]$$

where ν is an arbitrary constant. The nonlinear Fourier transform mentioned earlier can be obtained by performing the spectral analysis of eqn [5a]. The time evolution of the associated nonlinear Fourier data, which are now called spectral data, is linear and can be determined using eqn [5b]. Following Lax's formulation, Zakharov and Shabat (1972) solved the nonlinear Schrödinger (NLS) equation

$$\mathrm{i}q_t + q_{xx} - 2\lambda|q|^2 q = 0, \quad \lambda = \pm 1 \qquad [6]$$

which has ubiquitous physical applications including nonlinear optics. Soon thereafter the sine-Gordon equation

$$q_{xx} - q_{tt} = \sin q \qquad [7]$$

and the modified KdV equation

$$q_t + 6q^2 q_x + q_{xxx} = 0 \qquad [8]$$

were solved. Since then, numerous nonlinear equations have been solved. Thus, the mathematical technique introduced by Gardner *et al.* (1967) for the solution of a particular physical equation gave rise to a new method in mathematical physics, the so-called inverse-scattering (spectral) method. Among the most important equations solved by this method are a particular two-dimensional reduction of Einstein's equation and the self-dual Yang–Mills equations.

The next important development in the analysis of integrable equations was the study of the KdV with space-periodic initial data. This occurred in the mid-1970s in the USA and in the USSR. This method involves algebraic-geometric techniques; in particular there exists a periodic analog of the N-soliton solution which can be expressed in terms of a certain Riemann-theta function of genus N.

In the mid-1970s, it was also realized that there exist integrable ODEs. For example, a stationary reduction of some of the equations introduced in connection with the space-periodic problem mentioned above led to the integration of some classical tops. Furthermore, the similarity reduction of some of the integrable PDEs led to the classical Painlevé equations. For example, letting $q = t^{-1/3}u(\xi)$, $\xi = xt^{-1/3}$ in the modified KdV equation [8], and integrating we find

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + 2u^3 - \frac{1}{3}\xi u + \alpha = 0 \qquad [9]$$

where α is a constant. This is Painlevé II, that is, the second equation in the list of six classical ODEs introduced by Painlevé and is his school around 1900. These equations are nonlinear analogs of the linear special functions such as Airy, Bessel, etc. The connection between integrable PDEs and ODEs of the Painlevé type was established by Ablowitz and Segur (1977). Their work marked a new era in the theory of these equations. Indeed, soon thereafter Flaschka and Newell (1980) introduced an extension of the inverse-spectral method, the so-called isomonodromy method, capable of integrating these equations. The most remarkable achievement of this new development is the construction of nonlinear analogs of the classical connection formulas that exist for the linear special functions. These formulas, although rather complicated, are as explicit as the corresponding linear ones (Fokas *et al.* 2005).

It was mentioned earlier that the inverse-spectral method gives rise to a matrix RH problem. An RH problem involves the determination of a function analytic in given sectors of the complex plane, from the knowledge of the jumps of this function across the boundaries of these sectors. The algebraic-geometric method for solving the space-periodic initial-value problem can be interpreted as formulating an RH problem which can be analyzed using functions defined on a Riemann surface. Also, it was noted by Fokas and Ablowitz (1983a) and later rigorously established by Fokas and Zhou (1992) that the isomonodromy method also gives rise to a novel RH problem. This

implies the following interesting unification: Self-similar, decaying, and periodic initial-value problems for integrable evolution equations in one space variable lead to the study of the same mathematical object, namely to the RH problem.

Every integrable nonlinear evolution equation in one spatial dimension has several integrable versions in two spatial dimensions. Two such integrable physical generalizations of the Korteweg–deVries equation are the so-called Kadomtsev–Petviashvili I (KPI) and II (KPII) equations. In the context of water waves, they arise in the weakly nonlinear, weakly dispersive, weakly two-dimensional limit, and in the case of KPI when the surface tension is dominant. The NLS equation also has two physical integrable versions known as the Davey–Stewartson I (DSI), and II (DSII) equations. They can be derived from the classical water-wave problem in the shallow-water limit and govern the time evolution of the free surface envelope in the weakly nonlinear, weakly two-dimensional, nearly monochromatic limit. The KP and DS equations have several other physical applications.

A method for solving the Cauchy problem for decaying initial data for integrable evolution equations in two spatial dimensions emerged in the early 1980s. This method is sometimes referred to as the $\bar{\partial}$ (*d*-bar) method. We recall that the inverse-spectral method for solving nonlinear evolution equations on the line is based on a matrix RH problem. This problem expresses the fact that there exist solutions of the associated x-part of the Lax pair which are sectionally analytic. Analyticity survives in some multidimensional problems: it was shown formally by Fokas and Ablowitz (1983b) that KPI gives rise to a nonlocal RH problem. However, for other multidimensional problems, such as the KPII, the underlying eigenfunctions are nowhere analytic and the RH problem must be replaced by the $\bar{\partial}$ problem. Actually, a $\bar{\partial}$ problem had already appeared in the work of Beals and Coifman (1982) where the RH problem appearing in the analysis of one-dimensional systems was considered as a special case of a $\bar{\partial}$ problem. Soon thereafter, it was shown in Ablowitz *et al.* (1983) that KPII required the essential use of the $\bar{\partial}$ problem. The situation for the DS equations is analogous to that of the KP equations.

Multidimensional integral PDEs can support localized solutions. Actually there exist two types of localized coherent structures associated with integrable evolution equations in two spatial variables: the "lumps" and the "dromions." The spectral meaning, and therefore the genericity of these solutions was established by Fokas and Ablowitz (1983b) and Fokas and Santini (1990).

The analysis of integrable singular integro-differential equations and of integrable discrete equations, although conceptually similar to the analysis reviewed above, has certain novel features.

The fact that integrable nonlinear equations appear in a wide range of physical applications is not an accident but a consequence of the fact that these equations express a certain physical coherence which is natural, at least asymptotically, to a variety of nonlinear phenomena. Indeed, Calogero (1991) has emphasized that large classes of nonlinear evolution PDEs, characterized by a dispersive linear part and a largely arbitrary nonlinear part, after rescaling yield asymptotically equations (for the amplitude modulation) having a universal character. These "universal" equations are, therefore, likely to appear in many physical applications. Many integrable equations are precisely these "universal" models.

Solitons, Lumps, and Dromions

Solitons, lumps, and dromions, are important not because they are exact solutions, but because they characterize the long-time behavior of integrable evolution equations in one and two space dimensions. The question of solving the initial-value problem of a given integrable PDE, and then extracting the long-time behavior of the solution is quite complicated. It involves spectral analysis, the formulation of either an RH problem or of a $\bar{\partial}$ problem, and rigorous asymptotic techniques. On the other hand, having established the importance of solitons, lumps, and dromions, it is natural to develop methods for obtaining these particular solutions directly, avoiding the difficult approaches of spectral theory. There exist several such direct methods, including the so-called Bäcklund transformations, the dressing method of Zakharov–Shabat, the direct linearizing method of Fokas–Ablowitz, and the bilinear approach of Hirota.

Solitons

Using the bilinear approach, multisoliton solutions for a large class of integrable nonlinear PDEs in one space dimension are given in Hietarinta (2002). Here we only note that the 1-soliton solution of the NLS [6], of the sine-Gordon [7], and of the modified KdV equation [8] are given, respectively, by

$$q(x,t) = \frac{p_R e^{i(p_I x + (p_R^2 - p_I^2)t + \eta)}}{\cosh[p_R(x - 2p_I t) + \eta]} \qquad [10]$$

$$q(px + qt) = 4 \arctan[e^{px+qt+\eta}], \quad p^2 = 1 + q^2 \qquad [11]$$

$$q(x - p^2 t) = \frac{\pm p}{\cosh[px - p^2 t + \eta]} \qquad [12]$$

where p_R, p_I, η, p, q are real constants.

Lumps

The KPI equation is

$$\partial_x[q_t + 6qq_x + q_{xxx}] = 3q_{yy} \qquad [13]$$

The 1-lump solution of this equation is given by

$$\begin{aligned} q(x,y,t) &= 2\partial_x^2 \ln\left[|L(x,y,t)|^2 + \frac{1}{4\lambda_I^2}\right], \\ L &= x - 2\lambda y + 12\lambda^2 t + a \\ \lambda &= \lambda_R + \mathrm{i}\lambda_I, \quad \lambda_I > 0 \end{aligned} \qquad [14]$$

where λ and a are complex constants.

The focusing DSII equation is

$$\mathrm{i}q_t + q_{zz} + q_{\bar{z}\bar{z}} - 2q\left(\partial_{\bar{z}}^{-1}|q|_z^2 + \partial_z^{-1}|q|_{\bar{z}}^2\right) = 0 \qquad [15]$$

where $z = x + \mathrm{i}y$, and the operator $\partial_{\bar{z}}^{-1}$ is defined by

$$\left(\partial_{\bar{z}}^{-1} f\right)(z,\bar{z}) = \frac{1}{2\mathrm{i}\pi}\int_{\mathbb{R}^2} \frac{f(\zeta,\bar{\zeta})}{\zeta - z}\, \mathrm{d}\zeta \wedge \mathrm{d}\bar{\zeta}$$

The 1-lump solution of this equation is given by

$$q(z,\bar{z},t) = \frac{\beta \mathrm{e}^{\mathrm{i}(p^2+\bar{p}^2)t + pz - \bar{p}\bar{z}}}{|z + \alpha + 2\mathrm{i}pt|^2 + |\beta|^2} \qquad [16]$$

where α, β, p are complex constants. A typical 1-lump solution is depicted in **Figure 2**.

Dromions

The DSI equation is

$$\begin{aligned} \mathrm{i}q_t + \left(\partial_x^2 + \partial_y^2\right)q + qu &= 0 \\ u_{xy} &= 2\left(\partial_x^2 + \partial_y^2\right)|q|^2 \end{aligned} \qquad [17]$$

The 1-dromion solution of this equation is given by

$$\begin{aligned} q(x,y,t) &= \frac{\rho \mathrm{e}^{X - \bar{Y}}}{\alpha \mathrm{e}^{X+\bar{X}} + \beta \mathrm{e}^{-Y-\bar{Y}} + \gamma \mathrm{e}^{X+\bar{X}-Y-\bar{Y}} + \delta} \\ X &= px + \mathrm{i}p^2 t, \quad Y = qy + \mathrm{i}q^2 t \\ |\rho|^2 &= 4p_R q_R(\alpha\beta - \gamma\delta) \end{aligned} \qquad [18]$$

where p, q are complex constants and $\alpha, \beta, \gamma, \delta$ are positive constants.

A Nonlinear Fourier Transform

The solution of the initial-value problem of an integrable nonlinear evolution equation on the infinite line is based on the spectral analysis of the x-part of the Lax pair. Thus, for the KdV equation one must analyze eqn [5a]. This equation is the famous time-independent Schrödinger equation. We now give a physical interpretation of the relevant spectral analysis. Let KdV describe the propagation of a water wave and suppose that this wave is frozen at a given instant of time. By bombarding this water wave with quantum particles, one can reconstruct its shape from knowledge of how these particles scatter. In other words, the scattering data provide an alternative description of the wave at fixed time.

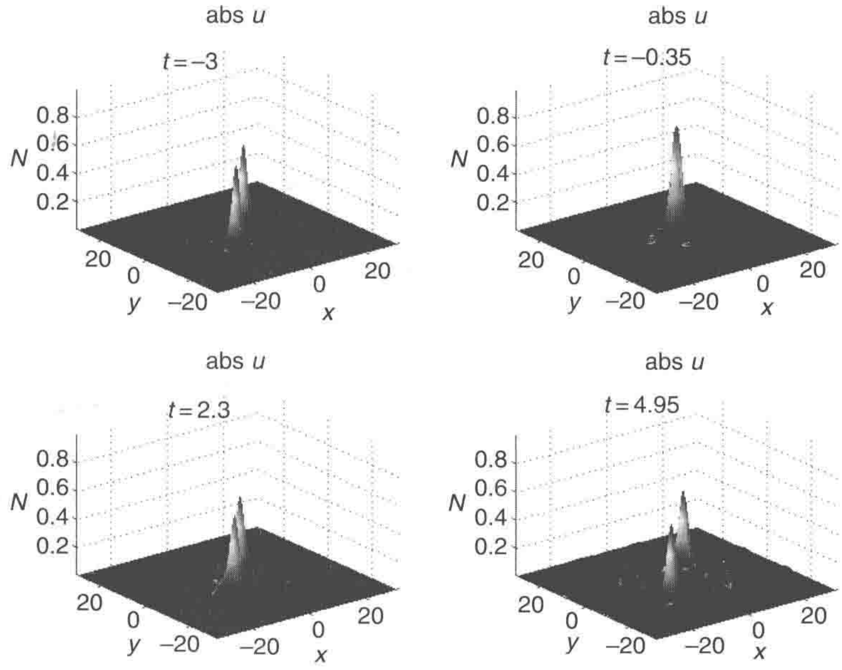


Figure 2 A typical 1-lump solution.

The mathematical expression of this description takes the form of a linear integral equation found by Faddeev (the so-called Gel'fand–Levitan–Marchenko equation) or equivalently the form of a 2×2 matrix RH problem uniquely specified by the scattering data. This alternative description of the shape of the wave will be useful if the evolution of the scattering data is simple. This is indeed the case, namely using eqn [5b], it can be shown that the scattering data evolve linearly. Thus, this highly nontrivial change of variables from the physical to scattering space provides a linearization of the KdV equation.

In what follows we will describe some of the relevant mathematical formulas. We first "assume" that there exists a real solution $q(x,t)$ of the initial-value problem which has sufficient smoothness and which decays for all t as $|x| \to \infty$. We then discuss how this assumption can be eliminated.

As it was mentioned earlier most of the analysis of the inverse-scattering transform is carried out on the x-part of the Lax pair, that is, on eqn [5a]. Hence, we first concentrate on eqn [5a] and for convenience of notation we suppress the time dependence.

The Direct Problem

As $|x| \to \infty, q \to 0$, thus there exist solutions of eqn [5a] which tend to $\exp[\pm ikx]$ as $|x| \to \infty$. Let $\psi(k,x)$ and $\hat{\psi}(k,x)$ denote solutions of eqn [5a] with the following asymptotic property:

$$\psi \to e^{ikx}, \quad \hat{\psi} \to e^{-ikx}, \quad \text{as } x \to \infty, \quad k \in \mathbb{R} \qquad [19]$$

Under the transformation $k \to -k$, eqn [5a] remains invariant and the boundary condition for ψ is mapped to the boundary condition for $\hat{\psi}$. Hence

$$\hat{\psi}(k,x) = \psi(-k,x) \qquad [20]$$

We denote by $\phi(k,x)$ the solution of eqn [5a] which tends to $\exp[-ikx]$ as $x \to -\infty$,

$$\phi \to e^{-ikx}, \quad \text{as } x \to -\infty, \quad k \in \mathbb{R} \qquad [21]$$

It is more convenient to work with eigenfunctions (i.e., solutions of [5a]) normalized to unity as $x \to \infty$, thus we introduce $M(k,x)$ and $N(k,x)$ as follows:

$$M = \phi e^{ikx}, \qquad N = \psi e^{-ikx} \qquad [22]$$

The functions M and N can be expressed in terms of q through the solution of linear Volterra integral equations. Indeed, M satisfies

$$M_{xx} - 2ikM_x = -qM, \quad k \in \mathbb{R}$$
$$M \to 1, \quad x \to -\infty \qquad [23]$$

The homogeneous version of [23] has solutions 1 and e^{2ikx}. Thus,

$$M = c_1 + c_2 e^{2ikx} + M_p \qquad [24]$$

where c_1, c_2 are constants and M_p is given by

$$M_p = u_1(x) + u_2(x) e^{2ikx} \qquad [25]$$

The functions u_1, u_2 satisfy

$$u_1' + e^{2ikx} u_2' = 0, \qquad 2ike^{2ikx} u_2' = -qM$$

Thus,

$$u_1(x) = \frac{1}{2ik} \int_{-\infty}^{x} d\xi q(\xi) M(k,\xi),$$
$$u_2(x) = -\frac{1}{2ik} \int_{-\infty}^{x} d\xi e^{-2ik\xi} q(\xi) M(k,\xi) \qquad [26]$$

Substituting [25] and [26] into [24] and using the boundary condition [23], we find

$$M(k,x) = 1 + \frac{i}{2k} \int_{-\infty}^{x} d\xi (-1 + e^{2ik(x-\xi)}) q(\xi) M(k,\xi) \qquad [27]$$

Similarly, one may establish that N satisfied

$$N(k,x) = 1 + \frac{i}{2k} \int_{x}^{\infty} d\xi (-1 + e^{-2ik(x-\xi)}) q(\xi) N(k,\xi) \qquad [28]$$

The kernel of eqn [27], as a function of k, is bounded and analytic for $\operatorname{Im} k > 0$. Thus, if $q \in L_1, M(k,x)$ as a function of k is holomorphic for $\operatorname{Im} k > 0$. Similarly, $N(k,x)$ as a function of k is holomorphic for $\operatorname{Im} k > 0$.

Thus, we have found particular solutions of eqn [5a] which are holomorphic for $\operatorname{Im} k > 0$. Furthermore, these solutions are simply related for k real. Indeed, the linear independence of solutions of the second-order ODE [5a] implies

$$\phi(k,x) = a(k)\hat{\psi}(k,x) + b(k)\psi(k,x), \quad k \in \mathbb{R}$$

Using [20] and replacing ϕ and ψ in terms of M and N, we find

$$\frac{M(k,x)}{a(k)} = N(-k,x) + \rho(k) e^{2ikx} N(k,x)$$
$$\rho(k) = \frac{b(k)}{a(k)}, \quad k \in \mathbb{R} \qquad [29]$$

The functions $a(k)$ and $b(k)$ are given by

$$a(k) = 1 - \frac{i}{2k}\int_{-\infty}^{\infty} d\xi q(\xi)M(k,\xi), \quad k \in \mathbb{R}$$
$$b(k) = \frac{i}{2k}\int_{-\infty}^{\infty} d\xi q(\xi)M(k,\xi)e^{-2ik\xi}, \quad k \in \mathbb{R} \qquad [30]$$

Indeed as $x \to \infty, N \to 1$, thus, eqn [29] implies

$$M \to a(k) + b(k)e^{2ikx} \text{ as } x \to \infty \qquad [31]$$

On the other hand, eqn [27] implies that

$$M \to 1 + \frac{i}{2k}\int_{-\infty}^{\infty} d\xi(-1 + e^{2ik(x-\xi)}q(\xi)M(k,\xi))$$
$$x \to \infty \qquad [32]$$

Comparing eqns [31] and [32], we find eqns [30].

The expression for $a(k)$ implies that this function is also holomorphic for $\operatorname{Im} k > 0$.

In summary, in the "direct problem," we have found particular solutions of eqn [5a] which are sectionally holomorphic:

$$\begin{pmatrix} M(k,x) \\ N(k,x) \end{pmatrix} \text{ and } \begin{pmatrix} M(-k,x) \\ N(-k,x) \end{pmatrix}$$

are holomorphic for $\operatorname{Im} k > 0$ and $\operatorname{Im} k < 0$, respectively. These solutions, which are characterized in terms of q by eqns [27] and [28], are simply related by eqn [29].

The Inverse Problem

Equation [28] expresses N in terms of q. Is it possible to find an alternative expression for N in terms of some appropriate "spectral data"? The answer is positive and is a direct consequence of the fact that eqn [29] defines the "jump condition" of an RH problem. Indeed, it can be shown that $a(k)$ may have simple zeros $k_1, \ldots, k_n$ in the positive imaginary axis of the k-complex plane. Hence, in general, M/a can be expressed in the form

$$\frac{M(k,x)}{a(k)} = \mathcal{M}(k,x) + \sum_{j=1}^{n} \frac{A_j(x)}{k - ip_j}, \quad p_j > 0$$

where $\mathcal{M}(k,x)$ as a function of k is holomorphic for $\operatorname{Im} k > 0$. It can also be shown that $A_j(x) = C_j \exp[-2p_j, x]N(k_j, x)$. Hence eqn [29] becomes

$$\mathcal{M}(k,x) - N(-k,x)$$
$$= \sum_{j=1}^{n} \frac{C_j e^{-2p_j x} N(ip_j, x)}{k - ip_j} + \rho(k)e^{2ikx}N(k,x), \quad k \in \mathbb{R}$$

Taking the $(-)$ projection of this equation, and using the fact that both $\mathcal{M}$ and N tend to 1 as $k \to \infty$, we find

$$N(k,x) - \frac{1}{2i\pi}\int_{-\infty}^{\infty} \frac{dl\rho(l)e^{2ilx}N(l,x)}{l + k + i0}$$
$$= 1 - \sum_{j=1}^{n} \frac{C_j e^{-2p_j x}}{k + ip_j} N(ip_j, x) \qquad [33]$$

In summary, this equation expressed $N(k,x)$ in terms of the scattering data $(\rho(k), \{C_j, p_j\}_1^n)$.

Since both eqns [28] and [33] are associated with the same q, these equations can be used to obtain the following expression for q:

$$q = -2\frac{\partial}{\partial x}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} dl\rho(l)e^{2ilx}N(l,x) - i\sum_{j=1}^{n} C_j e^{-2p_j x}N(ip_j, x)\right] \qquad [34]$$

Indeed, eqn [28] implies

$$\lim_{k\to\infty} N(k,x) = 1 - \frac{i}{2k}\int_{x}^{\infty} d\xi q(\xi)$$

Comparing this expression with the large-k behavior of eqn [33], we find [34].

Time Dependence of the Scattering Data

We now use eqn [5b] to compute the time dependence of the scattering data by evaluating eqn [5b] as $x \to -\infty$ we find $\nu = 4ik^3$. Then, evaluating it as $x \to \infty$ and using

$$\phi \sim ae^{-ikx} + be^{ikx}, \quad x \to +\infty$$

we find

$$a_t = 0, \qquad b_t = 8ik^3 b$$

Hence,

$$a(t,k) = a(0,k), \qquad \rho(t,k) = \rho(0,k)e^{8ik^3 t} \qquad [35]$$

Thus,

$$p_j(t) = p_j(0), \qquad C_j(t) = C_j(0)e^{8p_j^3 t} \qquad [36]$$

The above formal results motivate the following definitions (for simplicity, we assume that $a(k)$ has no zeros). Given a decaying real function

$q_0(x)$, $x \in \mathbb{R}$, define $M_0(k,x)$ as the solution of the linear Volterra integral equation

$$M_0(k,x) = 1 + \frac{i}{2k}\int_{-\infty}^{x} d\xi(-1 + e^{2ik(x-\xi)}q(\xi)M_0(k,\xi))$$
$$\operatorname{Im} k \geq 0$$

Given $M_0(k,x)$, define $a_0(k)$ and $b_0(k)$ by

$$M_0(k,x) \to a_0(k) + b_0(k)e^{2ikx}, \quad x \to \infty, \quad k \in \mathbb{R}$$

Given a_0 and b_0, define $N(k,x,t)$ by the solution of the linear integral equation

$$N(k,x,t) - \frac{1}{2\pi}\int_{-\infty}^{\infty} dl \frac{b_0(l)}{a_0(l)} e^{8il^3t+2ilx} \frac{N(l,x,t)}{l+k+i0} = 1$$

A theorem of Gohberg and Krein implies that this equation has a unique global solution. Given a_0, b_0, N, define $q(x,t)$ by

$$q(x,t) = -\frac{1}{\pi}\frac{\partial}{\partial x}\int_{-\infty}^{\infty} dk \frac{b_0(k)}{a_0(k)} e^{8ik^3t+2ikx} N(k,x,t)$$

Then it can be shown that $q(x,t)$ satisfies the KdV equation and $q(x,0) = q_0(x)$.

A Unification

After the emergence of a method for solving the initial-value problem for nonlinear integrable evolution equations in one and two space variables, the most outstanding open problem in the analysis of these equations became the solution of initial boundary-value problems. A general approach for solving such problems for evolution equations in one space dimension was provided by Fokas (1997). This approach has already been used for the study of nonlinear integrable evolution PDEs on the half-line (Fokas 2002, 2005), on the interval, and in a time-dependent domain. An important advantage of this new method is that it yields the formulation of a matrix RH problem (or a $\bar{\partial}$ problem in the case of a convex time-dependent domain), which although has more complicated jump matrices than the analogous problem on the infinite line, it still has an explicit exponential (x,t) dependence. This fact allows one to describe effectively the asymptotic properties of the solution, using the powerful Deift–Zhou method (Deift and Zhou 1993). For example, the long-time asymptotics of boundary-value problems on the half line are discussed in Fokas and Its (1996).

It is remarkable that the above results have motivated the discovery of a new method for solving boundary-value problems, not only for linear evolution PDEs, but also for linear elliptic PDEs in two dimensions. This includes the Laplace, the biharmonic and the Helmholtz equations in a convex polygon (Dassios and Fokas 2005). In a most recent development, this method has also been applied to certain classes of linear PDEs with variable coefficients. This highly unexpected development unifies and extends several classical branches of mathematics. In particular, it unifies the classical transform methods for simple linear PDEs as well as the method of images, the treatment of linear PDEs via certain ingenious techniques such as the Wiener–Hopf technique, the formulation of Ehrenpreis type integral representations, and the solution of integrable nonlinear PDEs via the inverse-scattering transform. Furthermore, it extends these results to arbitrary domains and to certain classes of PDEs with variable coefficients.

Regarding linear equations we note the following:

Almost as soon as linear two-dimensional PDEs made their appearance, d'Alembert and Euler discovered a general approach for constructing large classes of their solutions. This approach involved separating variables and superimposing solutions of the resulting ODEs. The method of separation of variables naturally led to the solution of PDEs by a transform pair. The prototypical such pair is the direct and the inverse Fourier transforms; variations of this fundamental transform include the Laplace, Mellin, sine, cosine transforms, and their discrete analogs.

The proper transform for a given boundary-value problem is specified by the PDE, by the domain, and by the given boundary conditions. For some simple boundary-value problems, there exists an algorithmic procedure for deriving the associated transform. This procedure involves constructing the Green's function of a single eigenvalue equation, and integrating this Green's function in the k-complex plane, where k denotes the eigenvalue.

The transform method has been enormously successful for solving a great variety of initial- and boundary-value problems. However, for sufficiently complicated problems the classical transform method fails. For example, there does not exist a proper analog of the sine transform for solving a third-order evolution equation on the half-line. Similarly, there do not exist proper transforms for solving boundary-value problems for elliptic equations even of second order and in simple domains. The failure of the transform method led to the development of several ingenious but *ad hoc* techniques, which include: conformal mappings for the Laplace and the biharmonic equations; the Jones method and the formulation of the Wiener–Hopf factorization problem; the use of some integral representation, such as that of Sommerfeld; the

formulation of a difference equation, such as the Malyuzhinet's equation. The use of these techniques has led to the solution of several classical problems in acoustics, diffraction, electromagnetism, fluid mechanics, etc. The Wiener–Hopf technique played a central role in the solution of many of these problems.

A crucial role in the new method is played by the global equation satisfied by the boundary values of q and of its derivatives. For evolution equations and for elliptic equations with simple boundary conditions, this involves the solution of a system of algebraic equations, while for elliptic equations with arbitrary boundary conditions, it involves the solution of an RH problem. For simple polygons, this RH problem is formulated on the infinite line, thus it is equivalent to a Wiener–Hopf problem. This explains the central role played by the Wiener–Hopf technique in many earlier works.

For linear PDEs, the explicit x_1, x_2 dependence of $q(x_1, x_2)$ is consistent with the Ehrenpreis formulation of the solution. Thus, this method provides the concrete implementation as well as the generalization to concave domains of this fundamental principle. For nonlinear equations, it provides the extension of the Ehrenpreis principle to integrable nonlinear PDEs.

See also: Boundary value Problems for Integrable Equations; $\bar{\partial}$-Approach to Integrable Systems; Integrable Systems and Algebraic Geometry; Integrable Discrete Systems; Integrable Systems and Discrete Geometry; Integrable Systems in Random Matrix Theory; Integrable Systems: Overview; Korteweg–de Vries Equation and Other Modulation Equations; Partial Differential Equations: Some Examples; Riemann–Hilbert Methods in Integrable Systems; Sine-Gordon Equation; Toda lattices; Twistor Theory: Some Applications [in Integrable Systems, Complex Geometry and String Theory].

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Integrable Systems in Random Matrix Theory

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Random Matrix Models

A random matrix model is a probability space $(\Omega, \mathcal{P}, \mathcal{F})$ where the sample space Ω is a set of matrices. There are three classic finite N random matrix models (see, e.g., Mehta (1991)):

1. Gaussian orthogonal ensemble ($\beta = 1$):
   (a) $\Omega = N \times N$ real symmetric matrices;
   (b) $\mathcal{P} =$ "unique" measure that is invariant under orthogonal transformations and the matrix elements are i.i.d. random variables; explicitly, the density is

$$c_N \exp(-\mathrm{tr}(A^2))\, \mathrm{d}A \qquad [1]$$

   where c_N is a normalization constant and $\mathrm{d}A = \prod_i \mathrm{d}A_{ii} \prod_{i<j} \mathrm{d}A_{ij}$, the product Lebesgue measure on the independent matrix elements.
2. Gaussian unitary ensemble ($\beta = 2$):
   (a) $\Omega = N \times N$ Hermitian matrices;
   (b) $\mathcal{P} =$ "unique" measure that is invariant under unitary transformations and the (independent) real and imaginary matrix elements are i.i.d. random variables; and
3. Gaussian symplectic ensemble ($\beta = 4$) (see Mehta (1991) for a definition).

Generally speaking, the interest lies in the $N \to \infty$ limit of these models. Here we concentrate on one aspect of this limit. In all three models the eigenvalues, which are random variables, are real and with probability 1 they are distinct. If $\lambda_{\max}(A)$ denotes the largest eigenvalue of the random matrix A, then for each of the three Gaussian ensembles we introduce the corresponding distribution function

$$F_{N,\beta}(t) := \mathrm{P}_\beta(\lambda_{\max} < t), \quad \beta = 1, 2, 4$$

The basic limit laws (see Tracy and Widom (1996) and references therein) state that

$$F_\beta(s) := \lim_{N\to\infty} F_{N,\beta}\Big(2\sigma\sqrt{N} + \frac{\sigma s}{N^{1/6}}\Big), \quad \beta = 1, 2, 4 \qquad [2]$$

exist and are given explicitly by

$$F_2(s) = \det(I - K_{\mathrm{Airy}}) = \exp\Big(-\int_s^\infty (x - s) q^2(x)\, \mathrm{d}x\Big)$$

where

$$K_{\mathrm{Airy}} \doteq \frac{\mathrm{Ai}(x)\mathrm{Ai}'(y) - \mathrm{Ai}'(x)\mathrm{Ai}(y)}{x - y}$$

acting on $L^2(s, \infty)$(Airy kernel)

and q is the unique solution to the Painlevé II equation

$$q'' = sq + 2q^3$$

satisfying the condition

$$q(s) \sim \mathrm{Ai}(s) \quad \text{as } s \to \infty$$

σ in eqn [2] is the standard deviation of the Gaussian distribution on the off-diagonal matrix elements. For the normalization we have chosen $\sigma = 1/\sqrt{2}$; however, for subsequent comparisons, the normalization $\sigma = \sqrt{N}$ is perhaps more natural.

The orthogonal and symplectic distribution functions are

$$F_1(s) = \exp\Big(-\frac{1}{2}\int_s^\infty q(x)\, \mathrm{d}x\Big)(F_2(s))^{1/2}$$

$$F_4(s/\sqrt{2}) = \cosh\Big(\frac{1}{2}\int_s^\infty q(x)\, \mathrm{d}x\Big)(F_2(s))^{1/2}$$

Graphs of the densities $\mathrm{d}F_\beta/\mathrm{d}s$ are in the adjacent figure and some statistics of F_β can be found in **Figure 1**.

The Airy kernel is an example of an integrable integral operator and a general theory is developed in Tracy and Widom (1994). A vertex operator approach to these distributions (and many other closely related distribution functions in random matrix theory) was initiated by Adler, Shiota, and van Moerbeke (see the review article var Moerbeke (2001) for further developments of this latter approach).

Historically, the discovery of the connection between Painlevé functions (P_{III} in this case) and Toeplitz/Fredholm determinants appears in work of Wu *et al.* (1976) on the spin–spin correlation functions of the two-dimensional Ising model. Painlevé functions first appear in random matrix theory in

β	μ_β	σ_β	S_β	K_β
1	−1.20653	1.2680	0.293	0.165
2	−1.77109	0.9018	0.224	0.093
4	−2.30688	0.7195	0.166	0.050

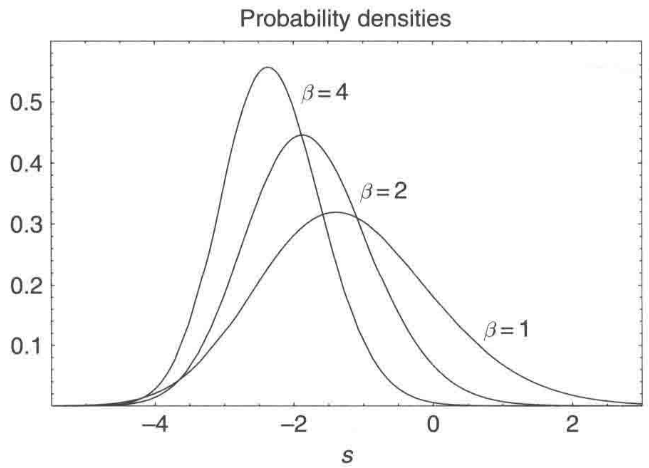


Figure 1 The mean (μ_β), standard deviation (σ_β), skewness (S_β), and kurtosis (K_β) of F_β.

Jimbo *et al.* (1980) where they prove that the Fredholm determinant of the sine kernel is expressible in terms of P_V. Gaudin (using Mehta's then newly invented method of orthogonal polynomials (Porter 1965)) was the first to discover the connection between random matrix theory and Fredholm determinants.

Universality Theorems

A natural question is to ask whether the above limit laws depend upon the underlying Gaussian assumption on the probability measure. To investigate this for unitarily invariant measures ($\beta = 2$), one replaces in [1]

$$\exp(-\mathrm{tr}(A^2)) \to \exp(-\mathrm{tr}(V(A)))$$

Bleher and Its (1999) choose

$$V(A) = gA^4 - A^2, \quad g > 0$$

and subsequently a large class of potentials V was analyzed by Deift *et al.* (1999). These analyses require proving new Plancherel–Rotach type formulas for nonclassical orthogonal polynomials. The proofs use Riemann–Hilbert methods. It was shown that the generic behavior is GUE; hence, the limit law for the largest eigenvalue is F_2. However, by finely tuning the potential new universality classes will emerge at the edge of the spectrum. For $\beta = 1, 4$ a universality theorem was proved by Stojanovic (2000) for the quartic potential.

In the case of noninvariant measures, Soshnikov (1999) proved that for real symmetric Wigner matrices (complex Hermitian Wigner matrices), the limiting distribution of the largest eigenvalue is F_1 (respectively, F_2). (A symmetric Wigner matrix is a random matrix whose entries on and above the main diagonal are independent and identically distributed random variables with distribution function F. Soshnikov assumes that F is even and all moments are finite.) The significance of this result is that non-Gaussian Wigner measures lie outside the "integrable class" (e.g., there are no Fredholm determinant representations for the distribution functions) yet the limit laws are the same as in the integrable cases.

Appearance of F_β in Limit Theorems

In this section we briefly survey the appearances of the limit laws F_β in widely differing areas.

Combinatorics

A major breakthrough occurred with the work of Baik, Deift, and Johansson (see Baik *et al.* (2000) and references therein) when they proved that the limiting distribution of the length of the longest increasing subsequence in a random permutation is F_2. Precisely, if $\ell_N(\sigma)$ is the length of the longest increasing subsequence in the permutation $\sigma \in S_N$, then

$$P\left(\frac{\ell_N - 2\sqrt{N}}{N^{1/6}} < s\right) \to F_2(s)$$

as $N \to \infty$. Here the probability measure on the permutation group S_N is the uniform measure. Further discussion of this result can be found in Johansson (2000b).

Baik and Rains (2001) showed by restricting the set of permutations (and these restrictions have natural symmetry interpretations) that F_1 and F_4 also appear. Even the distributions F_1^2 and F_2^2 (Tracy and Widom 1999) arise. By the Robinson–Schensted–Knuth correspondence, the Baik–Deift–Johansson result is equivalent to the limiting distribution on the number of boxes in the first row of random standard Young tableaux. (The measure is the push-forward of the uniform measure on S_N.) These same authors conjectured that the limiting distributions of the number of boxes in the second, third, etc., rows were the same as the limiting distributions of the next-largest, next-next-largest, etc., eigenvalues in GUE. Since these eigenvalue distributions were also found in Tracy and Widom (1996), they were able to compare the then unpublished numerical work of Odlyzko and Rains (2000) with the predicted results of random matrix theory. Subsequently, Baik *et al.* (2000) proved the conjecture for the second row. The full conjecture was proved by Okounkov (2000) using topological methods and by,

among others, Johansson (2001) using analytical methods. For an interpretation of the Baik–Deift–Johansson result in terms of the card game patience sorting, see the very readable review paper by Aldous and Diaconis (1999).

Growth Processes

Growth processes have an extensive history both in the probability literature and the physics literature (see, e.g., Meakin (1998) and references therein), but it was only recently that Johansson (2002b) proved that the fluctuations about the limiting shape in a certain growth model ("corner growth model") are F_2. Johansson further pointed out that certain symmetry constraints (inspired from the Baik and Rains (2001) work) lead to F_1 fluctuations (*see* Growth Processes in Random Matrix Theory).

Subsequently, Baik and Rains (2000) and Gravner *et al.* (2002) have shown the same distribution functions appearing in closely related lattice growth models. Prähofer and Spohn (2000) reinterpreted the work of Baik *et al.* in terms of the physicists' polynuclear growth (PNG) model thereby clarifying the role of the symmetry parameter β. For example, $\beta=2$ describes growth from a single droplet, whereas $\beta=1$ describes growth from a flat substrate. They also related the distribution functions F_β to fluctuations of the height function in the KPZ equation (Kardar *et al.* 1986, Meakin 1998). (The connection with the KPZ equation is heuristic.) Thus, one expects on physical grounds that the fluctuations of any growth process falling into the $1+1$KPZ universality class will be described by the distribution functions F_β or one of the generalizations by Baik and Rains (2000). Such a physical conjecture can be tested experimentally. Earlier Myllys *et al.* established experimentally that a slow, flameless burning process in a random medium (paper!) is in the $1+1$KPZ universality class. This sequence of events is a rare instance in which new results in mathematics inspire new experiments in physics.

In the context of the PNG model, Prähofer and Spohn have given a process interpretation, the Airy process, of F_2.

There is an extension of the growth model in Gravner *et al.* (2002) to growth in a random environment. In Gravner *et al.* (2002) the following model of interface growth in two dimensions is considered by introducing a height function on the sites of a one-dimensional integer lattice with the following update rule: the height above the site x increases to the height above $x-1$, if the latter height is larger; otherwise, the height above x increases by 1 with probability p_x. It is assumed that the p_x are chosen independently at random with a common distribution function F, and that the initial state is such that the origin is far above the other sites. In the pure regime, Gravner–Tracy–Widom identify an asymptotic shape and prove that the fluctuations about that shape, normalized by the square root of the time, are asymptotically normal. This contrasts with the quenched version: conditioned on the environment and normalized by the cube root of time, the fluctuations almost surely approach the distribution function F_2. We mention that these same authors find, under some conditions on F at the right edge, a composite regime where now the interface fluctuations are governed by the extremal statistics of p_x in the annealed case while the fluctuations are asymptotically normal in the quenched case.

Random Tilings

The Aztec diamond of order n is a tiling by dominoes of the lattice squares $[m,m+1]\times[\ell,\ell+1], m,n\in\mathbb{Z}$, that lie inside the region $\{(x,y):|x|+|y|\leq n+1\}$. A domino is a closed 1×2 or 2×1 rectangle in $\mathbb{R}^2$ with corners in $\mathbb{Z}^2$. A typical tiling is shown in **Figure 2**. One observes that near the center the tiling appears random, called the temperate zone, whereas near the edges the tiling is frozen, called the polar zones. As $n\to\infty$ the boundary between the temperate zone and the polar zones (appropriately scaled) converges to a circle ("arctic circle theorem"). Johansson (2002a) proved that the fluctuations about this limiting circle are F_2.

Statistics

Johnstone (2001) considers the largest principal component of the covariance matrix X^tX where X is an $n\times p$ data matrix all of whose entries are independent standard Gaussian variables and proves that for appropriate centering and scaling, the limiting distribution equals F_1 in the limit $n,p\to\infty$ with $n/p\to\gamma\in\mathbb{R}^+$. Soshnikov has removed the Gaussian assumption but requires that $n-p=O(p^{1/3})$. Thus, we can anticipate applications of the distributions F_β (and particularly F_1) to the statistical analysis of large data sets.

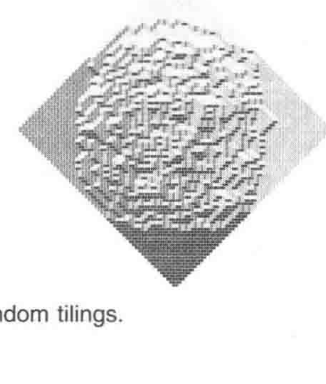


Figure 2 Random tilings.

Queuing Theory

Glynn and Whitt (1991) consider a series of n single-server queues each with unlimited waiting space with a first-in and first-out service. Service times are i.i.d. with mean one and variance σ^2 with distribution V. The quantity of interest is $D(k,n)$, the departure time of customer k (the last customer to be served) from the last queue n. For a fixed number of customers, k, they prove that

$$\frac{D(k,n)-n}{\sigma\sqrt{n}}$$

converges in distribution to a certain functional $\hat{D}_k$ of k-dimensional Brownian motion. They show that $\hat{D}_k$ is independent of the service time distribution V. It was shown in, for example, Gravner *et al.* (2002) that $\hat{D}_k$ is equal in distribution to the largest eigenvalue of a $k \times k$ GUE random matrix. This fascinating connection has been greatly clarified in recent work of O'Connell and Yor (2002).

From Johansson (2002), it follows for V Poisson that

$$P\left(\frac{D(\lfloor xn \rfloor, n) - c_1 n}{c_2 n^{1/3}} < s\right) \to F_2(s)$$

as $n \to \infty$ for some explicitly known constants c_1 and c_2 (depending upon x).

Superconductors

Vavilov *et al.* (2001) have conjectured (based upon certain physical assumptions supported by numerical work) that the fluctuation of the excitation gap in a metal grain or quantum dot induced by the proximity to a superconductor is described by F_1 for zero magnetic field and by F_2 for nonzero magnetic field. They conclude their paper with the remark:

> The universality of our prediction should offer ample opportunities for experimental observation.

Acknowledgments

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See also: Determinantal Random Fields; Growth Processes in Random Matrix Theory; Integrable Systems and Algebraic Geometry; Integrable Systems and the Inverse Scattering Method; Integrable Systems: Overview; Quantum Calogero–Moser Systems; Random Partitions; Random Matrix Theory in Physics; Symmetry Classes in Random Matrix Theory; Toeplitz Determinants and Statistical Mechanics.

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Integrable Systems: Overview

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Introduction

This section introduces some elementary notions and sets the (mathematically low brow) tone of this presentation.

A *dynamical system* is characterized by an evolution equation the general structure of which reads

$$Q_t = F \quad [1]$$

Here $Q \equiv Q(x,t)$ is the dependent variable, and it might be a scalar, a vector, a matrix, you name it. The focus of interest is on its evolution as function of the (real, scalar) "time" variable t. The *a priori* unknown quantity Q might moreover depend on another independent "space" variable (scalar or vector) x, $Q \equiv Q(x,t)$. The appended variable t in the left-hand side of the above equation denotes partial differentiation, and this notation will be used throughout, although when t is the only independent variable differentiation with respect to it might be instead denoted by a superimposed dot:

$$Q_t \equiv \frac{\partial Q(x,t)}{\partial t}, \; Q_x \equiv \frac{\partial Q(x,t)}{\partial x}, \; \dot{Q} \equiv \frac{dQ(t)}{dt}$$

The quantity in the right-hand side of the evolution equation (1), which has of course the same (scalar, vector, matrix) character as Q, is an *assigned* function of t, x and Q, $F \equiv (x,t,Q)$ (more generally, its dependence on Q might be functional, see below). A typical example of the dynamical systems we shall consider is the N-body problem characterized by the Newtonian equations of motion

$$\ddot{q}_n = -\omega^2 q_n + 2g^2 \sum_{m=1, m\neq n}^{N} (q_n - q_m)^{-3}, \; n = 1, 2, \ldots N \quad [2]$$

where the dependent variable is the N-vector $\vec{q} \equiv (q_1, \ldots q_N)$, the components of which are the "particle coordinates" $q_n \equiv q_n(t)$. Note however that these equations of motion are of *second-order* in time (contrary to (1)); but they can of course be reformulated as *first-order* ODEs indeed their Hamiltonian version, derived in the standard manner from the Hamiltonian

$$H = \frac{1}{2}\sum_{n=1}^{N}(p_n^2 + \omega^2 q_n^2) + \frac{g^2}{2}\sum_{m,n=1;m\neq n}^{N}(q_n - q_m)^{-2} \quad [3a]$$

reads

$$\dot{q}_n = p_n \quad [3b]$$

$$\dot{p}_n = -\omega^2 q_n + 2g^2 \sum_{m=1, m\neq n}^{N} (q_n - q_m)^{-3}, \; n = 1, 2, \ldots N \quad [3c]$$

Other typical examples are the ("Korteweg-de Vries", "Burgers", "Nonlinear Schrödinger", "sine Gordon") PDEs satisfied by the scalar dependent variable $q \equiv q(x,t)$,

$$q_t = -q_{xxx} + 2q_x q = \left(-q_{xx} + q^2\right)_x \quad [4]$$

$$q_t = -q_{xx} + 2q_x q = \left(-q_x + q^2\right)_x \quad [5]$$

$$q_t = i\left[q_{xx} + s|q|^2 q\right], \; s = \pm \quad [6]$$

$$q_t - q_x = s, s_t + s_x = \sin q \quad [7]$$

as well as the integrodifferential ("Benjamin–Ono") equation

$$q_t = P\int_{-\infty}^{\infty} dy \frac{q_{yy}(y)}{x-y} + q_x q \quad [8]$$

and the ("Kadomtsev–Petviashvili") PDE satisfied by the scalar dependent variable $q \equiv q(x, y, t)$,

$$q_{tx} = (-q_{xxx} + q_x q)_x + s q_{yy}, \; s = \pm \quad [9]$$

This last equation should of course be reformulated as an integrodifferential equation to fit with (1).

These are all examples of *integrable systems* (see below). In this presentation we restrict attention to dynamical systems of these general types, without considering evolutions in which the space variable, and/or the time variable, and/or the dependent variable, only take discrete values, forsaking thereby the discussion of discrete evolution equations, cellular automata and functional equations, see other entries of this Encyclopedia. We shall consider mainly the "initial-value problem" in which the solution is assigned at the initial time, say at $t=0$,

$$Q(x, 0) = Q_0(x)$$

and the subsequent evolution of the dependent variable, namely the values taken by $Q(x,t)$ for $t > 0$, is the focus of attention. Note however that, except when there is no dependence at all on the space variable x (see for instance (2)), the functional class to which $Q(x,t)$ belongs as regards its x-dependence should be specified (and the assigned initial-value $Q_0(x)$ should of course belong to this functional class). A typical class of functions are those vanishing (adequately fast) at (spatial) infinity; another typical class are those characterized by periodicity properties as functions of x; and still another class are those restricted to a finite spatial domain (for instance, the positive x-axis, $x > 0$, or a finite interval, $a \le x \le b$), in which cases the initial-value problem must be supplemented by assigning boundary conditions. These latter class of problems, called initial/boundary-value problems, are generally more difficult; even the identification of which boundary conditions are adequate to identify uniquely the solution may be a nontrivial task. In the following we will always focus on the simpler class of problems characterized by solutions defined in the entire space region and vanishing (sufficiently fast) asymptotically (far away).

Thus, in the spirit of the initial-value problem, a dynamical system is generally characterized by assigning its evolution equation, the functional class to which its solutions are required to belong, and possibly in addition some (additional) restriction on the set of initial data.

Let us finally mention that, aside from considering the initial-value problem, the study of dynamical systems may focus on the identification of special (classes of) solutions, for instance those obtained by using symmetry properties of the evolution equation under consideration (yielding, say, "similarity solutions"), and, in the integrable case, "solitonic" and "multisolitonic" solutions (see below).

Integrable dynamical systems

The solution of a dynamical system, however simple the equation that defines its time evolution, see (1), may be extremely complicated, indeed its time-dependence might feature one or more of the characteristics of *deterministic chaos*, such as a *sensitive dependence* on the initial data. But there are "exceptional" dynamical systems, the behavior of which is instead, in some sense, *simple*. Such systems are termed – in the least technical sense of the word – "integrable".

This characterization can be made precise for Hamiltonian systems with a finite number N of degrees of freedom, the equations of motion of which read

$$\dot{q}_n = \frac{\partial H(\vec{p},\vec{q})}{\partial p_n}, \dot{p}_n = -\frac{\partial H(\vec{p},\vec{q})}{\partial q_n}, n = 1, \ldots N$$

Such a system is *integrable* if there exist, in addition to the Hamiltonian $H(\vec{p},\vec{q}) \equiv H^{(1)}(\vec{p},\vec{q})$ itself, $N-1$ other (nontrivial and functionally independent) constants of motion $H^{(m)}(\vec{p},\vec{q})$ *in involution*, namely such that their Poisson brackets vanish:

$$\begin{aligned}&\left\{H^{(n)}, H^{(m)}\right\}\\ &\quad \equiv \sum_{\ell=1}^{N}\left[\frac{\partial H^{(n)}(\vec{p},\vec{q})}{\partial q_\ell}\frac{\partial H^{(m)}(\vec{p},\vec{q})}{\partial p_\ell}\right.\\ &\qquad \left. - \frac{\partial H^{(m)}(\vec{p},\vec{q})}{\partial q_\ell}\frac{\partial H^{(n)}(\vec{p},\vec{q})}{\partial p_\ell}\right] = 0,\\ &\quad n, m = 1, \ldots, N\end{aligned}$$

Let us however emphasize the crucial role of the words "there exist", as used just above. For definiteness let us require that the constants of motion $H^{(n)}(\vec{p},\vec{q})$ be *analytic functions* of their $2N$ arguments, and *not excessively multivalued*: they might feature some branch points, but not so many to vanify their effectiveness in constraining the time evolution of the dynamical variables $q_n(t), p_n(t)$ sufficiently to avoid their behavior from being too complicated. On the other hand it is of course not necessary that these functions $H^{(n)}(\vec{p},\vec{q})$ be *explicitly* known.

When these conditions hold it is in principle possible ("Liouville theorem") to identify a

canonical transformation from the canonical coordinates and momenta q_n and p_n to *action-angle variables* θ_n and I_n such that

$$I_n = H^{(n)}(\vec{p}, \vec{q}) \qquad [10]$$

Then these action variables evolve trivially,

$$I_n(t) = I_n(0), \theta_n(t) = \theta_n(0) + I_n(0)t, n = 1, \ldots N$$

Note that, once these new canonical variables are identified, the solution of the initial-value problem for the original Hamiltonian problem is provided directly by the expressions of the action-angle variables θ_n and I_n in terms of the original variables q_n and p_n, as well as the expressions of the latter in terms of the former. The second step of this procedure requires inverting the expressions (10), and the corresponding expressions of the angle variables θ_n in terms of the original variables q_n and p_n; a necessary condition in order that this step allow to identify uniquely, at least in principle, the original canonical variables q_n and p_n in terms of the action-angle variables I_n and θ_n – hence imply a *simple* time-evolution of these original variables – is the requirement, as mentioned above, that the expressions of the constants of the motion $H^{(n)}(\vec{p}, \vec{q})$ in terms of their arguments q_n and p_n not be excessively multivalued.

The statements outlined above can be rigorously formulated for finite-dimensional Hamiltonian systems, and they can be heuristically extended to all analogous dynamical systems with a finite number of degrees of freedom, even if they are not Hamiltonian.

A system with N degrees of freedom might possess more than N constants of motion. Such a system that possesses $2N - 1$ (nontrivial and functionally independent) constants of motion (the maximal number, to avoid the evolution being frozen) is called *superintegrable*, and its evolution is in some sense analogous to that of a system with a single degree of freedom, in particular *all* its *confined* and *nonsingular* motions are then *completely periodic*,

$$q_n(t + T) = q_n(t), p_n(t + T) = p_n(t), n = 1, \ldots, N$$

The period T depends generally on the initial data. If it does not, at least for an open set of such data having full dimensionality in phase space, the system is called *isochronous*: *all* its motions in that phase space region are then *completely periodic with the same period*.

A dynamical system might be integrable in a region of its "natural" phase space, and nonintegrable in another region. Sometimes such systems are referred to as *partially integrable*. There even are systems which are *isochronous* (hence *superintegrable*) in a region of their phase space, and behave instead *chaotically* in another region. These regions are generally separated by boundaries where the evolution of the system runs into singularities, and the constants of motion associated with the integrable behavior become *excessively multivalued* in the regions where the behavior is *chaotic*. (*see* Isochronous Systems).

Dynamical systems featuring an additional space variable x (see Section 1) can be interpreted as *infinite-dimensional* dynamical systems (by considering the variable x as a continuous label for the dependent variable Q). Accordingly, a necessary condition in order that such systems be considered *integrable* is the requirement that they possess an *infinite* number of constants of the motion. But – even for such systems that allow a Hamiltonian formulation – this condition cannot be considered sufficient (due to the inherent ambiguities in the counting of infinities), and in fact a completely cogent, universally accepted definition of *integrability* for infinite-dimensional dynamical systems is still lacking (various definitions can of course be given in special contexts). It is nevertheless rather well understood by practitioners what is meant by such a term at least for *integrable* equations such as those indicated at the end of the previous section, which generally give rise to the *solitonic* phenomenology – as explained below.

The study of integrable systems has an illustrious history, to which many eminent mathematicians and mathematical physicists contributed after the Newtonian revolution: Euler, Jacobi, Poincaré, Painlevé, Kowalewskaya, Kolmogorov, Moser ... Below we report – most tersely – on the bloom that this topic has witnessed over the last 3–4 decades, without being generally able, due to space constraints, to attribute the appropriate credit to the many colleagues, most of them still living, who contributed to this endeavor. For more detailed treatments of the topics outlined below, of related developments not mentioned here, and of such credits, the interested reader is referred to the bibliography given below, including the additional references traceable from there.

Integrable many-body problems

An important class of integrable dynamical systems is provided by N-body problems characterized by Hamiltonians such as

$$H(\vec{p}, \vec{q}) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + V(\vec{q}) \qquad [11]$$

with a potential energy $V(\vec{q})$ that includes "external" and "two-body" forces,

$$V(\vec{q}) = \sum_{n=1}^{N} V^{(1)}(q_n) + \frac{1}{2}\sum_{m,n=1;m\neq n}^{N} V^{(2)}(q_n - q_m),$$
$$V^{(2)}(-q) = V^{(2)}(q) \qquad [12]$$

The corresponding Hamiltonian and Newtonian equations of motion read

$$\dot{q}_n = p_n, \dot{p}_n = -\frac{\partial V^{(1)}(q_n)}{\partial q_n} - \sum_{m=1, m\neq n}^{N} \frac{\partial V^{(2)}(q_n - q_m)}{\partial q_n},$$

$$\ddot{q}_n = -\frac{\partial V^{(1)}(q_n)}{\partial q_n} - \sum_{m=1, m\neq n}^{N} \frac{\partial V^{(2)}(q_n - q_m)}{\partial = q_n} \qquad [13]$$

The Lax pair and the constants of motion Suppose that two $N \otimes N$ matrices $L \equiv L(\vec{p}, \vec{q})$ and $M \equiv M(\vec{p}, \vec{q})$ could be found such that the matrix "Lax equation"

$$\dot{L} = [L, M] \qquad [14]$$

be equivalent to the Hamiltonian equations of motion (13). Here and throughout the notation $[A, B]$ denotes the commutator:

$$[A, B] \equiv A\,B - B\,A$$

Because this matrix equation clearly entails that the N traces

$$T_n = \text{trace}\,[L^n], n = 1, \ldots, N$$

are constants of the motion,

$$\dot{T}_n = 0, n = 1, \ldots, N$$

the possibility to write the Hamiltonian equations (13) in the Lax form (14) yields as a bonus N constants of the motion, namely it entails that the Hamiltonian system under consideration is *integrable*. (One must moreover show that these constants of motion are *in involution*; this is usually the case).

Hence a route to identify *integrable* N-body problems is via the search of Lax pairs L, M of matrices such that (14) correspond to (13), with an appropriate assignment of the potential energy (12). For $N > 2$ this is a nontrivial task, because (13) is a system of $2N$ ODEs in $2N$ unknowns, while the matrix Lax equation (14) amounts to a system of N^2 ODEs.

Functional equations and the identification of integrable many-body problems A convenient *ansatz* to identify a *Lax pair* suitable for the purpose outlined above reads as follows:

$$L_{nm} = p_n \text{ for } n = m, L_{nm} = \alpha(q_n - q_m) \text{ for } m \neq n,$$

$$M_{nm} = \sum_{\ell=1, \ell\neq n}^{N} \beta(q_n - q_\ell) \text{ for } n = m,$$

$$M_{nm} = \gamma(q_n - q_m), \text{ for } m \neq n$$

where $\alpha(q), \beta(q)$ and $\gamma(q)$ are 3 functions to be determined. It is then easily seen that these functions may be assigned so that the corresponding Lax equation (14) be equivalent to the Hamiltonian equations (13) with

$$V^{(1)}(q) = 0 \qquad [15a]$$

$$V^{(2)}(q) = \alpha(q)\alpha(-q) \qquad [15b]$$

provided the function $\alpha(x)$ satisfies the *functional equation*

$$\frac{\alpha(x)\alpha'(y) - \alpha(y)\alpha'(x)}{\alpha(x + y)} = \beta(x) - \beta(y), \beta(x) = \beta(-x)$$

The general solution of this functional equation yields via [15b] the two-body potential

$$V^{(2)}(q) = g^2 a^2 \wp(a\,q|\omega, \omega') \qquad [16]$$

where g and a are two arbitrary constants and $\wp(x|\omega, \omega')$ is the Weierstrass elliptic function (with semiperiods ω and ω', as well arbitrary). One concludes therefore that the N-body problem characterized by the Hamiltonian (11) with (12), (15a) and (16) is *integrable*.

This Hamiltonian system has played, since the mid-seventies, a seminal role in the developments of finite-dimensional integrable systems that occurred over the last few decades. However, since the Weierstrass function is doubly-periodic, from a "physical" point of view this N–body problem is rather unrealistic, or perhaps rather suited for the study of crystalline configurations, including their statistical mechanics. But there are two special cases, obtained by assigning an infinite value to one or both of the semiperiods of the Weierstrass function in (16), that qualify $V^{(2)}(q)$ as a physical two-body potential:

$$V^{(2)}(q) = \frac{g^2 a^2}{\sinh^2(a\,q)} \qquad [17a]$$

$$V^{(2)}(q) = \frac{g^2}{q^2} \qquad [17b]$$

(Of course the second of these two-body potentials, (17b), is merely the special case of the first, (17b), corresponding to $a = 0$). These Hamiltonian models are then naturally interpretable as one-dimensional many-body problems with repulsive two-body forces singular at zero separation and vanishing at large distances. Actually the fact that these systems are *integrable* is far from remarkable, since it is generally true that any many-body problem characterized by repulsive forces vanishing at large distances (hence causing *unconfined* motions) is *integrable*: indeed in such models the particles eventually separate and move freely, so that their trajectories cannot display the extreme complication

characterizing a *chaotic* (i.e., *nonintegrable*) behavior. But these models are in fact *superintegrable* and they (as well as various *integrable* extensions of them) feature many (physically and mathematically) interesting properties. For instance the asymptotic behavior of their trajectories,

$$q_n(t) = p_n^{(\pm)}t + q_n^{(\pm)} + o(1), p_n(t) = p_n^{(\pm)} + o(1)$$
$$\text{as } t \to \pm\infty, n = 1, \ldots, N \quad [18]$$

is characterized by the simple rules

$$p_n^{(+)} = p_{N+1-n}^{(-)}, n = 1, \ldots, N,$$
$$q_n^{(+)} = q_n^{(-)} + \sum_{m=1, m\neq n}^{N} \Delta\left(p_m^{(-)} - p_n^{(-)}; g, a\right) \quad [19]$$
$$n = 1, \ldots, N$$

with

$$\Delta(p; g, a) = \text{sign}(p)\frac{\log\left[1 + (ga/p)^2\right]}{2a}$$

The formula (19) indicates that the shift $q_n^{(+)} - q_n^{(-)}$ among the asymptotic positions of the particles (see (18)) is merely a sum of *two-body* shifts Δ (which incidentally vanish altogether if $a = 0$, namely in the (17b) case), and it only depends on the velocities $p_n^{(-)}$ of the particles in the remote past (*not* on the corresponding asymptotic positions $q_n^{(-)}$, in spite of their relevance in determining the order in which the different particles approach each other through the motion).

A generalization of the above model in the (17b) case – nontrivial inasmuch as it yields *confined* motions – is characterized by the additional presence in the potential (12) of the one-body potential

$$V^{(1)}(q) = \tfrac{1}{2}\,\omega^2 q^2 \quad [20]$$

yielding the Hamiltonian (3a). This model is *integrable*, indeed *superintegrable*, indeed *isochronous*, all its (real) solutions being *completely periodic* with period

$$T = \frac{2\pi}{\omega} \quad [21]$$

A neat way to understand this result is by noting that, if $\tilde{q}(t)$ is a (possibly *complex*) solution of the model discussed above (in this subsection, with the two-body potential (17b) and no one-body potential, see (15a)), then

$$q_n(t) = \exp(-i\omega t)\tilde{q}_n(\tau), \tau = \frac{\exp(2\,i\omega t) - 1}{2\,i\omega}$$

provides a (possibly *real*) solution of the Newtonian equations of motion (2), namely of the same model but with the additional one-body potential (20). Remarkably this model was solved firstly in the quantal case (at the beginning of the seventies), and only a few years later in the classical case considered here (by J. Moser, who, for the $\omega = 0$ case, introduced the special version of the Lax matrix appropriate for this case).

Another class of many-body problems, introduced in the mid-sixties by M. Toda, played a seminal role in the study of *integrable* dynamical systems, indeed the first application (independently by H. Flaschka and S. Manakov) of the Lax approach to *integrable* many-body problems occurred in that context. This model is often referred to as the Toda lattice, because its (two-body) interaction (of exponential type) is only assumed to act among "nearest neighbors".

A particularly interesting, and just as integrable, generalization of this class of Hamiltonian many-body problems features an extra parameter, say c, which might be considered to play the role of "speed of light". These models reduce to those considered above for $c = \infty$, and for finite c they are invariant under the Poincaré group of coordinate transformations (while of course the many-body problems described above are invariant under the Galilei group). They are sometimes termed RS models, to recognize those who first introduced them (S. Ruijsenaars and H. Schneider) as well as the possibility to interpret them in some sense as "relativistic" generalizations of the "nonrelativistic" models described above.

Reduction of the solution to algebraic operations The solution of the models described above can actually be reduced to purely algebraic operations. For instance for the model characterized by the Newtonian equations of motion (2) such a solution of the initial-value problem is provided by the following prescription: the particle coordinates $q_n(t)$ coincide with the N eigenvalues of the $N \otimes N$ matrix:

$$\tilde{Q}_{nm}(t) = q_n(0)\cos(\omega t) + \dot{q}_n(0)\frac{\sin(\omega t)}{\omega} \quad \text{for } n = m,$$
$$\tilde{Q}_{nm}(t) = \frac{ig\,\sin(\omega t)}{\omega[q_n(0) - q_m(0)]} \quad \text{for } n \neq m$$

Many-body problems related to the motion of the zeros of linear PDEs Another convenient approach to manufacture and investigate *integrable* many-body problems is by identifying the motion of the particles with that of the zeros of (polynomial)

solutions of linear (hence solvable) evolution PDEs. Assume for instance that the monic polynomial

$$\psi(z,t) = x^N + \sum_{m=1}^{N} c_m(t) x^{N-m} = \prod_{n=1}^{N} [z - z_n(t)] \quad [22]$$

satisfies the (compatible) linear PDE

$$\begin{aligned}&[A_0 + A_1 z + A_2 z^2 + A_3 z^3]\psi_{zz} \\ &+ [B_0 + B_1 z - 2(N-1)A_3 z^2]\psi_z \\ &+ C\psi_{tt} + [E - (N-1)D_2 z]\psi_t \\ &+ [D_0 + D_1 z + D_2 z^2]\psi_{zt} \\ &- [N(N-1)(A_2 - A_3 z) + NB_1]\psi = 0 \quad [23]\end{aligned}$$

where the letters $A_0, A_1, A_2, A_3, B_0, B_1, C, D_0, D_1, D_2, E$ denote 11 arbitrary constants. Then the zeros $z_n(t)$ evolve according to the system of ODEs

$$\begin{aligned}C\ddot{z}_n + E\dot{z}_n &= B_0 + B_1 z_n - 2(N-1)A_3 z_n^2 \\ &+ \sum_{m=1, m\neq n}^{N} (z_n - z_m)^{-1} \\ &\times [2C\dot{z}_n\dot{z}_m - (\dot{z}_n + \dot{z}_m)(D_0 + D_1 z_n) \\ &- D_2 z_n(\dot{z}_n z_m + \dot{z}_m z_n) \\ &+ 2(A_0 + A_1 z_n + A_2 z_n^2 + A_3 z_n^3)] \quad [24]\end{aligned}$$

interpretable as the Newtonian equations of motion of an N-body problem with one- and two-body (velocity-dependent) forces. This problem is *integrable*, indeed its solution can be reduced to the algebraic problem of finding the zeros of the polynomial $\psi(z,t)$, see (22), whose time evolution can be ascertained by solving the linear PDE (23), itself a purely algebraic problem as it amounts to solving the system of (constant coefficients, linear) ODEs implied via (22) by this PDE (23) for the N coefficients $c_m(t)$.

This class of many-body problems is rather rich, thanks to the arbitrariness of the 11 constants it features. Several subcases, characterized by special choices of these constants, are suitable to display a gamut of different phenomenological behaviors: confined and nonconfined motions, periodic and nonperiodic evolutions, limit cycles, Hamiltonian cases, ...

Solvable many-body problems in the plane The many-body problems considered above were all essentially *one-dimensional*. But via a simple trick it is possible to obtain from some of them *many-body problems in the plane* (which should of course be *rotation-invariant* to be certified as such). Consider for instance the special case of the above model, (24), with $C=1$ and with $A_0 = A_1 = A_3 = B_0 = D_0 = D_2 = 0$ so that its equations of motion,

$$\begin{aligned}\ddot{z}_n + E\dot{z}_n &= B_1 z_n + \sum_{m=1, m\neq n}^{N} (z_n - z_m)^{-1} \\ &\times [2\dot{z}_n\dot{z}_m - D_1(\dot{z}_n + \dot{z}_m)z_n + 2A_2 z_n^2] \quad [25]\end{aligned}$$

are invariant under rescaling of the dependent variables ($z_n \Longrightarrow cz_n$). Let us then assume to work in the *complex* rather than the *real*, and let us set

$$E = \gamma + i\omega,\ A_2 = \alpha + i\tilde{\alpha},\ B_1 = \beta + i\tilde{\beta},\ D_1 = \delta + i\tilde{\delta}$$

where the Greek letter indicate now *real* constants, and let us moreover relate the N complex coordinates z_n to N two-vectors $\vec{r}_n$ in the horizontal plane via the self-evident positions

$$z_n = x_n + iy_n, \vec{r}_n = (x_n, y_n, 0); \hat{k} = (0,0,1) \quad [26]$$

It is then easily seen that the *integrable* equations of motion (25) become the following *rotation-invariant* Newtonian equations of motion identifying a (no less *integrable*) N-body problem *in the plane*:

$$\begin{aligned}&\ddot{\vec{r}}_n + \left(\gamma + \omega\hat{k}\wedge\right)\dot{\vec{r}}_n \\ &= \left(\beta + \tilde{\beta}\hat{k}\wedge\right)\vec{r}_n + \sum_{m=1, m\neq n}^{N} r_{nm}^{-2} \\ &\left[2\left\{\dot{\vec{r}}_n\left(\dot{\vec{r}}_m\cdot\vec{r}_{nm}\right) + \dot{\vec{r}}_m\left(\dot{\vec{r}}_n\cdot\vec{r}_{nm}\right) - \vec{r}_{nm}\left(\dot{\vec{r}}_n\cdot\dot{\vec{r}}_m\right)\right\}\right. \\ &- \left(\delta + \tilde{\delta}\hat{k}\wedge\right)\left\{\left(\dot{\vec{r}}_n + \dot{\vec{r}}_m\right)[r_n^2 - (\vec{r}_n\cdot\vec{r}_m)]\right. \\ &\left. - \vec{r}_n\left[\vec{r}_m\cdot\left(\dot{\vec{r}}_n + \dot{\vec{r}}_m\right)\right] + \vec{r}_m\left[\vec{r}_n\cdot\left(\dot{\vec{r}}_n + \dot{\vec{r}}_m\right)\right]\right\} \\ &\left. + 2\left(\alpha + \tilde{\alpha}\hat{k}\wedge\right)\left\{\vec{r}_n[r_n^2 - 2(\vec{r}_n\cdot\vec{r}_m)] + \vec{r}_m r_n^2\right\}\right] \quad [27]\end{aligned}$$

Here and below we use the short-hand notation $\vec{r}_{nm} = \vec{r}_n - \vec{r}_m$ entailing $r_{nm}^2 = r_n^2 + r_m^2 - 2\vec{r}_n\cdot\vec{r}_m$, the symbol $\wedge$ denotes the three-dimensional vector product so that $\hat{k}\wedge\vec{r}_n = (-y_n, x_n, 0)$ (see (26)), and the rest of the notation is self-evident. Note that these *rotation-invariant* Newtonian equations of motion are also *translation-invariant* if $\beta = \tilde{\beta} = \delta = \tilde{\delta} = \alpha = \tilde{\alpha} = 0$.

The "goldfish" model The attribute of "goldfish" has been attributed to the special case of the above model with *all* "coupling constants" vanishing, thanks to the neatness of its equations of motion, which in their *complex* version read

$$\ddot{z}_n = 2\sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m}{z_n - z_m}, n = 1, \ldots, N$$

and in their *real* ("physical") version as Newtonian equations of motion of an N-body problem in the horizontal plane read

$$\ddot{\vec{r}}_n = 2 \sum_{m=1, m \neq n}^{N} \frac{\dot{\vec{r}}_n \left(\dot{\vec{r}}_m \cdot \vec{r}_{nm}\right) + \dot{\vec{r}}_m \left(\dot{\vec{r}}_n \cdot \vec{r}_{nm}\right) - \vec{r}_{nm} \left(\dot{\vec{r}}_n \cdot \dot{\vec{r}}_m\right)}{r_{nm}^2}$$
$$n = 1, \ldots, N$$

(This name has also been attributed to some extensions of this model, see the entry *Isochronous Systems* in this Encyclopedia). This model is invariant under time rescaling ($t \Rightarrow ct$), in its physical version it is *translation-* and *rotation-invariant*, it only features *two-body* forces and in spite of their *velocity-dependence* it is *Hamiltonian* (it is in fact a simple instance of the RS models mentioned above). The solution of its initial-value problem (in its *complex* version) is given by a remarkably neat rule: the N coordinates $z_n(t)$ are the N roots of the following algebraic equations in z:

$$\sum_{n=1}^{N} \frac{\dot{z}_n(0)}{z - z_n(0)} = \frac{1}{t} \qquad [28]$$

The phenomenology of its *generic* solution is also remarkable, corresponding to the "game of musical chairs": in the remote past all particles but one are *almost* at rest in $N-1$ positions ("sitting in $N-1$ chairs") and one particle comes in from infinity, moving initially as a free particle; as it approaches, all the particles begin to move around ("dancing"); in the remote future one particle goes away (moving eventually with the same speed as the incoming particle), and all the others settle down in the same $N-1$ positions ("of the $N-1$ chairs"), but with the possibility that the outgoing particle be different from the incoming one, and that the other particles have reshuffled their "seating".

Another remarkable version (also *translation-* and *rotation-invariant*, as well as *Hamiltonian*) of the N-body model in the plane (27) obtains if all the "coupling constants" vanish except ω. Then *all* its *nonsingular* solutions – which are given by the same prescription indicated just above, except for the replacement of $\frac{1}{t}$ with $\frac{i\omega}{\exp(i\omega t)-1}$ in the right-hand side of (28) – are *completely periodic* with periods which are an integer multiple – no larger than a number depending on N, generally (much) smaller than $N!$ – of T (see (21)), the domains of phase space that give rise to solutions with different periodicity being separated from each other by boundaries characterized by lower-dimensional sets of initial data yielding trajectories that run into *singularities* corresponding to *particle collisions* (note that when two or more particles collide their individuality gets lost, and their velocities diverge).

Integrable many-body problems in spaces with arbitrary dimensions *Integrable*, or even *solvable*, many-body problems in spaces with more than two dimensions – with *rotation-invariant* equations of motion of Newtonian type – can be manufactured by starting from an appropriate *integrable*, or *solvable*, second-order *matrix* evolution equation, and by then parametrizing the evolving matrix in terms of multidimensional vectors so as to transform the matrix evolution equation into a *covariant* – hence *rotation-invariant* – system of evolution equations for these vectors, interpretable as Newtonian equations of motion of a many-body problem in multidimensional space.

For instance the matrix equation

$$\dot{M} = AM + MA + M^3$$

is *integrable*. Here $M \equiv M(t)$ is a square matrix of arbitrary order and A is an *arbitrary* constant matrix. By parametrizing appropriately these two matrices one concludes that either one of the following two Newtonian systems of ODEs is *integrable*:

$$\ddot{\vec{r}}_{nm} = \sum_{\nu=1}^{N} \alpha_{n\nu} \vec{r}_{\nu m} + \sum_{\mu=1}^{M} \sum_{\nu=1}^{N} \vec{r}_{n\mu} \left(\vec{r}_{\nu\mu} \cdot \vec{r}_{\nu m}\right)$$
$$n = 1, \ldots, N, m = 1, \ldots, M,$$
$$\ddot{\vec{r}}_{nm} = \sum_{\nu=1}^{N} \alpha_{n\nu} \vec{r}_{\nu m} + \sum_{\mu=1}^{M} \sum_{\nu=1}^{N} \vec{r}_{\nu\mu} \left(\vec{r}_{\nu\mu} \cdot \vec{r}_{nm}\right)$$
$$n = 1, \ldots, N, m = 1, \ldots, M.$$

Here N and M are *arbitrary* positive integers, the NM constants α_{nm} are also *arbitrary*, the NM "particle coordinates" $\vec{r}_{nm} \equiv \vec{r}_{nm}(t)$ are S-vectors, with S an *arbitrary* positive integer, and the dots sandwiched among these S-vectors denote the standard scalar product in S-dimensional space.

Let us emphasize the physical relevance of this class of many-body problems, characterized by *linear* and *cubic* forces. This is reinforced by the fact that these models are *Hamiltonian*.

Nonlinear harmonic oscillators Two classes of *integrable* systems obtain from the classes written above by first setting to zero all the constants α_{nm} and by then performing the change of variables

$$\vec{w}_{nm}(t) = \exp(i\omega t)\vec{r}_{nm}(\tau), \tau = \frac{\exp(i\omega t) - 1}{i\omega} \qquad [29]$$

with $\omega > 0$. The corresponding Newtonian equations of motion read

$$\ddot{\vec{w}}_{nm} - 3i\omega\dot{\vec{w}}_{nm} - 2\vec{w}_{nm} = \sum_{\mu=1}^{M}\sum_{\nu=1}^{N} \vec{w}_{n\mu}(\vec{w}_{\nu\mu} \cdot \vec{w}_{\nu m})$$
$$n = 1, \ldots, N, m = 1, \ldots, M,$$
$$\ddot{\vec{w}}_{nm} - 3i\omega\dot{\vec{w}}_{nm} - 2\vec{w}_{nm} = \sum_{\mu=1}^{M}\sum_{\nu=1}^{N} \vec{w}_{\nu\mu}(\vec{w}_{\nu\mu} \cdot \vec{w}_{nm})$$
$$n = 1, \ldots, N, m = 1, \ldots, M$$

These equations of motion cause the $N\,M$ evolving S-vectors $\vec{w}_{nm} \equiv \vec{w}_{nm}(t)$ to be *complex* (see the second term in their left-hand sides), but a *real* system (with double the number of dependent variables) can be easily obtained by setting

$$\vec{w}_{nm} = \vec{u}_{nm} + i\vec{v}_{nm}$$

Remarkably (but clearly suggested by (29)), *all* the *nonsingular* solutions of each of these two many-body problems are *completely periodic*, with a period which is an integer multiple of the period T, see (21). This justifies the title given to this subsection. It also shows that these are *isochronous systems* (*see* Isochronous Systems).

Integrable nonlinear PDEs

As indicated in Section 1 another class of integrable systems are nonlinear evolution PDEs. In this section we outline (some of) their properties, focussing mainly on the Korteweg-de Vries PDE (4), the solution of which by C. S. Gardner, J. M. Greene, M. D. Kruskal and R. M. Miura in the mid-sixties was the opening shot of a major scientific development which is still blooming. Other important early steps of this development were, in the late sixties, the introduction by P. D. Lax of what is now called the Lax pair technique, and at the beginning of the seventies the solution by V. E. Zakharov and A. B. Shabat of the Nonlinear Schrödinger equation (6) – an evolution PDE of great applicative importance. Subsequently many researchers developed various techniques to identify, classify and investigate *integrable* nonlinear PDEs, a continuing activity for an overall appraisal of which the interested reader is referred to the bibliography reported below.

Here we outline one of the approaches to obtaining these results; other approaches are tersely mentioned below.

Identification and investigation of integrable PDEs via the inverse spectral transform technique

The class of *linear dispersive* evolution PDEs reads

$$u_t(x,t) = -i\omega\left(-i\frac{\partial}{\partial x}\right)u(x,t), -\infty < x < \infty \quad [30]$$

where the "dispersion function" $\omega(z)$ is, say, a (*real*) polynomial (which must be *odd* to guarantee that this PDE be *real*). The solution of this PDE is achieved via the introduction of the Fourier transform $\hat{u}(k,t)$,

$$u(x,t) = (2\pi)^{-1}\int_{-\infty}^{\infty} dk \exp(i\,kx)\,\hat{u}(k,t) \quad [31a]$$

$$\hat{u}(k,t) = \int_{-\infty}^{\infty} dx \exp(-i\,kx)u(x,t) \quad [31b]$$

whose evolution corresponding to (30) is then given by the simple linear ODE

$$\hat{u}_t(k,t) = -i\omega(k)\hat{u}(k,t), -\infty < k < \infty \quad [32a]$$

which can be immediately integrated:

$$\hat{u}(k,t) = \hat{u}(k,0)\exp[-i\omega(k)t] \quad [32b]$$

Thus the solution of the initial-value problem of (30) is achieved via three steps: (i) at the initial time one obtains the initial value of the Fourier transform, $\hat{u}(k,0)$, from the initial datum $u(x,0)$ (via (31b)); (ii) one then obtains $\hat{u}(k,t)$ (via (32b)); (iii) one finally obtains $u(x,t)$ (via (31a)). From these formulas the main features of the resulting phenomenology are easily evinced (even when the above integrals cannot be explicitly performed).

A class of *integrable nonlinear* evolution PDEs reads

$$u_t(x,t) = \alpha(\mathbf{R})u_x(x,t) \quad [33]$$

where the assigned function $\alpha(z)$ is again, say, a (*real*) polynomial, while $\mathbf{R}$ is now the integrodifferential "recursion operator" defined by the following formula that specifies its action on a generic function $f(x,t)$ (vanishing asymptotically so as to allow all integrations to converge):

$$\mathbf{R}f(x,t) = f_{xx}(x,t) - 4u(x,t)f(x,t) + 2u_x(x,t)\int_x^{\infty} dy\,f(y,t) \quad [34]$$

Note that the presence of the time variable t plays no relevant role (it is merely parametric). A remarkable property of this operator – which depends on $u(x,t)$ – is that any power of it acting

on $u_x(x,t)$ yields a nonlinear combination of $u(x,t)$ and its x-derivatives – without any left-over integration, in fact yielding a result which is itself an exact x-derivative, ready for exact integration in case of a further application of **R**, see the last term in the right-hand side of (34). For instance

$$\mathbf{R}u_x = u_{xxx} - 6u_x u = \left(u_{xx} - 3u^2\right)_x,$$
$$\mathbf{R}^2 u_x = u_{xxxxx} - 10u_{xxx}u - 20u_{xx}u_x + 30u_x u^2 = \left(u_{xxxx} - 10u_{xx}u - 5u_x^2 + 10u^3\right)_x$$

and so on. Hence the simplest nonlinear evolution equation contained in the class (33) is the Korteweg-de Vries (KdV) equation

$$u_t + u_{xxx} = 6u_x u \qquad [35]$$

(corresponding to $\alpha(z) = -z$; and note the identity with (4), via the trivial rescaling $q(x,t) = 3\,u(x,t)$). Note that, if one neglects all nonlinear contributions, the class (33) reduces to (30) with

$$\omega(z) = -z\alpha(-z^2)$$

The solution of this class of *nonlinear* PDEs, (33), is given by a somewhat analogous procedure to that described above for the class of *linear* dispersive PDEs (30).

Firstly, one introduces the *spectral transform*, a nonlinear generalization of the Fourier transform which indeed reduces to it if nonlinear effects are altogether neglected. That relevant for the class of PDEs (33) is based on the spectral problem associated with the linear Schrödinger operator

$$\mathbf{L} = -\left(\frac{\partial}{\partial x}\right)^2 + u(x,t), -\infty < x < \infty \qquad [36]$$

Via it, the spectral transform

$$S[u(x,t)] = \{R(k,t), -\infty < k < \infty; p_n, \rho_n(t), n = 1,\ldots,N\} \qquad [37]$$

is introduced. Here the function $R(k,t)$ is the "reflection coefficient" associated to the eigenvalue k^2 of the *continuous* spectrum of **L**, while the nonnegative number N gives the number of *discrete* eigenvalues of **L**, and the positive quantities p_n and $\rho_n(t)$ are associated to these discrete eigenvalues, specifically $-p_n^2$ are the "binding energies", and $\rho_n(t)$ the "normalization coefficients", associated to the "bound states" possessed by the "potential" $u(x,t)$. (All this terminology comes from the interpretation of the above spectral problem in quantum-mechanical terms). And it can be shown not only that there is a one-to-one correspondence among a function $u(x,t)$ and its spectral transform $S[u(x,t)]$, but moreover that both the *direct spectral problem* to compute $S[u(x,t)]$ from $u(x,t)$ (arbitrarily assigned within an appropriate class), and the *inverse spectral problem* to compute $u(x,t)$ from $S[u(x,t)]$ (arbitrarily assigned within an appropriate class), only entail solving *linear* equations (an ODE in the former case, a Fredholm integral equation in the latter case).

Note that, in the above definition of the spectral transform, the time variable t plays merely a parametric role. But the usefulness of this spectral transform to solve the PDE (33) resides in the fact that, if $u(x,t)$ evolves in time according to this PDE, the corresponding evolution of the spectral transform is quite simple: the number N and the positive numbers p_n are time-independent (as already implied by our notation), while the time evolution of the reflection coefficient $R(k,t)$ and of the normalization coefficients $\rho_n(t)$ is given by the simple *linear* ODEs

$$R_t(k,t) = 2ik\alpha(-4k^2)R(k,t), -\infty < k < \infty \qquad [38a]$$

$$\dot\rho_n(t) = -2p_n\alpha(4p_n^2)\rho_n(t), n = 1,\ldots,N \qquad [38b]$$

which can be readily integrated:

$$R(k,t) = R(k,0)\exp\left[2ik\alpha(-4k^2)t\right] \qquad [39a]$$

$$\rho_n(t) = \rho_n(0)\exp\left[-2p_n\alpha(4p_n^2)t\right] \qquad [39b]$$

Hence the solution of the initial-value problem for the class of nonlinear PDEs (33) can now be achieved via the following three steps: (i) at the initial time, via the solution of the *direct spectral problem*, the spectral transform $S[u(x,0)]$ (see (37)) is obtained (from $u(x,0)$, arbitrarily assigned within an appropriate class); (ii) the spectral transform at time t is then obtained via (39); (iii) by solving the *inverse spectral problem*, $u(x,t)$ is obtained from $S[u(x,t)]$ (see (37)).

The analogy of this procedure to that outlined above for the class of linear dispersive PDEs (30) is clear, and the fact that in this manner the solution of the initial-value problem for the nonlinear PDEs (33) can be achieved via a sequence of steps involving only the solution of *linear* problems is an indication of the *integrable* character of this class of *nonlinear* evolution PDEs. And it allows to gain thereby a lot of insight on the behavior of these solutions, and also to construct classes of explicit solutions of these equations, as we now indicate.

Solitons

The *integrable* nonlinear PDE (33) possesses the *single-soliton* solution

$$u(x,t) = \frac{-2p^2}{\cosh^2\{p[x-\xi(t)]\}} \qquad [40a]$$

$$\xi(t) = (2p)^{-1}\log\left[\frac{\rho(t)}{2p}\right] = \xi(0) + vt,$$
$$v = -\alpha(4p^2) \qquad [40b]$$

to which corresponds the simple *spectral transform*

$$S[u(x,t)] = \{R(k,t) = 0; p_1 = p,$$
$$\rho_1(t) = \rho(t) = \rho(0)\exp[-2p\alpha(4p^2)t]; N = 1\} \qquad [41]$$

This solution, (40), describes a localized wave of constant shape moving with the constant speed v: the "soliton". It is characterized by two (*real*) parameters, $\xi(0)$ and p. The first identifies the initial location of the *soliton*; its arbitrariness corresponds to the translation invariant character of (33). The second, p, the spectral significance of which is clear from (41), determines the shape of the *soliton* (both its "height" $2p^2$ and its "width" $\frac{1}{p}$) as well as its speed v (see (40b)); note that the shape is identical for all the nonlinear evolution PDEs of the class (33), while the speed depends on the function $\alpha(z)$, see (40b), namely it depends on which specific equation of the class (33) one is considering. For instance for the KdV equation (35), corresponding to $\alpha(z) = -z$, the speed of the soliton is

$$v = 4p^2 \qquad [42]$$

thus *all* solitons of the KdV equation move from left to right, and taller and thinner solitons move faster than less tall and more fat ones.

More generally, every PDE of the class (33) possesses the N-soliton solution

$$u(x,t) = -2\left(\frac{\partial}{\partial x}\right)^2 \log\det[\mathbf{I} + \mathbf{C}(x,t)] \qquad [43a]$$

Here $\mathbf{I}$ is the $N \otimes N$ unit matrix and $\mathbf{C}(t)$ is the $N \otimes N$ matrix

$$C_{mn}(x,t) = [\rho_m(t)\rho_n(t)]^{1/2}\frac{\exp[-(p_m+p_n)x]}{p_m+p_n} \qquad [43b]$$

where the time-evolution of the $\rho_n(t)$'s is given by (39b). Indeed the spectral transform of this solution is given by (37) with $R(k,t)=0$ and $\rho_n(t)$ given by (39b). To discuss the multisolitonic phenomenology, let us focus on the KdV equation, so that the speed of each soliton is given by the simple formula (42) and let us order the N positive numbers p_n in increasing order,

$$p_1 < p_2 < \cdots < p_N$$

so that the corresponding soliton velocities, $v_n = 4p_n^2$, are as well ordered in increasing order:

$$v_1 < v_2 < \cdots < v_N$$

The N-soliton solution (43) is not so transparent, especially if N is large, but it becomes quite simple in the remote past and future:

$$u(x,t) \approx \sum_{n=1}^{N} \frac{-2p_n^2}{\cosh^2\{p_n[x-\xi_n(t)]\}},$$
$$\xi_n(t) = \xi_n^{(\pm)} + v_n t, t \to \pm\infty$$

with the $2N$ (*real*) constants $\xi_n^{(\pm)}$ related to one another (see below). It is thus seen that, both in the remote past and future, the N-soliton solution (43) splits into the sum of N separated solitons. In the remote past the solitons are ranged, from left to right, in order of decreasing amplitude, and they move to the right with speeds ordered in decreasing magnitude; then the taller and faster solitons gradually catch up and eventually "overtake" the fatter and slower ones (the quotation marks underscore the fact that whenever two, or possibly more, solitons get together, their individuality is in fact lost: for a while the solution might have just one peak, or instead the "overtaking" of two solitons may rather appear as an "exchange of identity", with the taller soliton becoming fatter and the fatter becoming taller as they get close together until they separate again because the one in front, having become taller, speeds up while the one behind, having become fatter, slows down). The final outcome is of course that the order of the solitons gets altogether reversed, with the taller and faster heading the escape to the right. The most remarkable aspect of this phenomenology is that precisely the same solitons that existed in the remote past are found in the remote future, the only effect of their "interaction" having been to shift the position of the *n-th* soliton, relative to what it would have been if it had been moving in isolation, by the amount

$$\Delta_n = \xi_n^{(+)} - \xi_n^{(-)}$$

These N shifts are moreover determined (while either the N quantities $\xi_n^{(-)}$ or the N quantities $\xi_n^{(+)}$ can be arbitrarily assigned), being given by the simple rule

$$\Delta_n = \sum_{m=1}^{n-1}\Delta(p_n,p_m) - \sum_{m=n+1}^{N}\Delta(p_n,p_m) \qquad [44a]$$

$$\Delta(p_n, p_m) = \frac{1}{p_n} \log\left(\frac{p_n + p_m}{|p_n - p_m|}\right) \qquad [44b]$$

Of course in (44a) a sum vanishes if its lower limit exceeds its upper limit.

This formula (44), has a simple phenomenological significance. From the two-soliton case ($N = 2$) it is seen that in a *two-body* encounter the taller and faster soliton gets *advanced* by the amount $\Delta(p_2, p_1)$, while the slower and fatter one gets *delayed* by the amount $\Delta(p_1, p_2)$. Hence the overall shift (44) experienced by the n-th soliton in the N-soliton case is the sum of the $n - 1$ positive shifts derived from its "overtaking" $n - 1$ slower solitons and the $N - n$ negative shifts derived from its being "overtaken" by $N - n$ faster solitons. This outcome is obvious when each two-soliton encounter occurs *separately*, but is quite nontrivial in the general case when, at some intermediate time, several solitons might all encounter simultaneously.

This soliton phenomenology strongly suggest ascribing to each soliton an individuality, even though in configuration space it only shows up as a separate entity in the remote past and future. The separated identity of each soliton is instead quite clear in the spectral transform context, since each of them corresponds to a (time-independent) discrete eigenvalue of the spectral problem. Indeed in the spectral context this identity is clear also for the generic solution of the class of integrable nonlinear PDEs (33) which, in contrast to the purely solitonic solution (43), is *not* characterized by a vanishing reflection coefficient $R(k, t)$. And indeed, even in configuration space, the soliton phenomenology described above is still featured by a *generic* solution (each of which is characterized, via its spectral transform (37), by the number N of its solitons), up to the additional presence of a "background" component of this solution (corresponding to the nonvanishing reflection coefficient $R(k, t)$), which however behaves in a manner analogous to the solution of the linear, dispersive part of the PDE under consideration, becoming eventually locally small due to its dispersive character.

Kinks, breathers, boomerons and trappons, dromions The solitonic phenomenology described above for the class of integrable PDEs (33), and in particular for the KdV equation (35), is more or less common to all *integrable* nonlinear evolution PDEs – of which many other classes exist besides (33). But there also are some significant differences, some of which we now review tersely.

For certain *integrable* PDEs the typical shape of the soliton is not localized, but it rather has the form of a "kink". Some *integrable* PDEs also feature additional kinds of localized "solitons" which, in isolation, move overall with constant speed as ordinary solitons, but feature in addition a time-dependent amplitude modulation and are therefore called "breathers". For *integrable* matrix nonlinear evolution PDEs – or, equivalently, for *integrable* systems of coupled PDEs – the new phenomenology may emerge of solitons that, even in isolation, move with a variable speed, the change of which over time is correlated with the variable interplay of the amplitudes of the different components of the solution: typically such solitons come in from one side in the remote past and boomerang back to that side in the remote future ("boomerons"), or they may be trapped to oscillate around some fixed position ("trappons"); and there are *integrable* evolution equations in which both these types of solitons are simultaneously present in a generic solution. All these phenomenologies refer to the simpler class of *integrable* evolution PDEs in $1 + 1$ (one space and one time) variables, with asymptotically vanishing boundary conditions (at large space distances; or perhaps asymptotically constant, as in the case of kinks). There also exist *integrable* evolution PDEs in $2 + 1$ dimensions (such as the KP equation (9)) the generic solution of which may feature localized soliton-like components, although in this case appropriate boundary conditions play a crucial role (for this reason such solitons have been called "dromions", hinting at their being to some extent driven by the boundary conditions, as objects moving in a stadium).

While there are quite many (classes of) integrable PDEs in $1 + 1$ dimensions, there are only a few in $2 + 1$ dimensions, and there is a widespread belief that no integrable PDEs exist in $D + 1$ dimensions with $D > 2$. But already in the early days of soliton theory it was pointed out that there do exist quite many (classes of) integrable PDEs in $1 + D$ dimensions (namely, one space and D time variables) and that it is quite possible via a different formulation of the initial-value problem to interpret such equations as (no less *integrable*) PDEs in $D + 1$ dimensions (D space and one time variables); and *integrable* PDEs in $D + 1$ dimensions have also been identified and investigated in the context of (the simpler class of) *C-integrable* PDEs (see below).

Other properties of integrable PDEs

For the *linear* evolution equations (30) the main message implied by their solvability via the Fourier transform is, that the time-evolution is much simpler in Fourier space (see (32)) than in configuration

space. This has a profound impact on the understanding of all phenomena describable by such equations, to the extent of determining the kind of experimental tools better suited to understand the underlining physics (for instance, the use of monochromatic beams of light, the use of high-energy particle accelerators, and so on). The same kind of message is as well relevant for the class of *integrable* nonlinear PDEs solvable via the spectral transform technique – even more so inasmuch as the time-evolution is in this case so much simpler in the spectral space (being actually *linear* there, see (38) and (39)) than in configuration space (where the evolution is *nonlinear*, see (33)). It is indeed the basis for the possession by the class of *integrable* nonlinear PDEs (33) of several other remarkable properties as outlined tersely in the following subsections.

Bäcklund transformations A Bäcklund transformation is a formula relating two functions, say $u^{(0)}(x,t)$ and $u^{(1)}(x,t)$, so that, if one of them satisfies a (generally nonlinear) PDE, the other one satisfies the same PDE. In the context of the class (33) of *integrable* PDEs, such a (class of) Bäcklund transformations is provided by the formula

$$g(\Lambda)\left[u^{(0)}(x,t)-u^{(1)}(x,t)\right]+h(\Lambda)\Gamma\,1=0 \qquad [45]$$

where $g(z)$ and $h(z)$ are two (*a priori* arbitrary) entire functions (say, two polynomials), while Λ and Γ are two integrodifferential operators the effect of which on a function $f(x,t)$ (such that all relevant integrations are convergent) reads

$$\begin{aligned}\Gamma f(x,t)=&\left[u_x^{(0)}(x,t)+u_x^{(1)}(x,t)\right]f(x,t)\\&+\left[u^{(0)}(x,t)-u^{(1)}(x,t)\right]\\&\times\int_x^{\infty}dy\left[u^{(0)}(y,t)-u^{(1)}(y,t)\right]f(y,t)\end{aligned} \qquad [46a]$$

$$\begin{aligned}\Lambda f(x,t)=&f_{xx}(x,t)-2\left[u^{(0)}(x,t)+u^{(1)}(x,t)\right]f(x,t)\\&+\Gamma\int_x^{\infty}dyf(y,t)\end{aligned} \qquad [46b]$$

Note that here the variable t plays no relevant role (its presence is merely parametric), and that Γ and Λ depend (in a symmetrical way) on $u^{(0)}(x,t)$ and $u^{(1)}(x,t)$, whose presence causes the Bäcklund transformation (45) to be *nonlinear* in these functions. Also important is the observation that, for $u^{(0)}(x,t)=u^{(1)}(x,t)=u(x,t)$, the operator Λ becomes the recursion operator **R**, see (34).

The reason why the formulas (45) constitute a class of Bäcklund transformations is because – as a property of the spectral transform based on the linear Schrödinger operator L, see (36) – if two "potentials" $u^{(0)}(x,t)$ and $u^{(1)}(x,t)$ are related by (45), the corresponding "reflection coefficients" $R^{(0)}(k,t)$ and $R^{(1)}(k,t)$ are related *algebraically*, as follows:

$$\begin{aligned}&g(-4k^2)\left[R^{(0)}(k,t)-R^{(1)}(k,t)\right]\\&\quad+2ikh(-4k^2)\left[R^{(0)}(k,t)+R^{(1)}(k,t)\right]=0\end{aligned} \qquad [47a]$$

entailing

$$R^{(1)}(k,t)=R^{(0)}(k,t)\frac{g(-4k^2)+2ikh(-4k^2)}{g(-4k^2)-2ikh(-4k^2)} \qquad [47b]$$

Clearly this formula entails that, if $R^{(0)}(k,t)$ satisfies (38a), so does $R^{(1)}(k,t)$. Hence, as the fact that $R^{(0)}(k,t)$ satisfies (38a) is a consequence of the fact that $u^{(0)}(x,t)$ satisfies (33), likewise the fact that $R^{(1)}(k,t)$ satisfies (38a) provides the basis for concluding that $u^{(1)}(x,t)$ also satisfies (33).

The simpler version of the Bäcklund transformation (45) obtains by setting $g(z)=-2ph(z)$ with p an arbitrary constant, hence it reads

$$\begin{aligned}&w_x^{(0)}(x,t)+w_x^{(1)}(x,t)\\&\quad=2p\left[w^{(0)}(x,t)-w^{(1)}(x,t)\right]\\&\qquad-\frac{1}{2}\left[w^{(0)}(x,t)-w^{(1)}(x,t)\right]^2\end{aligned} \qquad [48]$$

Here and below we use for convenience the functions $w^{(j)}(x,t)$ related to $u^{(j)}(x,t)$ as follows:

$$\begin{aligned}w^{(j)}(x,t)&=\int_x^{\infty}dy\,u^{(j)}(y,t),\\w_x^{(j)}(x,t)&=-\,u^{(j)}(x,t)\end{aligned} \qquad [49]$$

A convenient application of Bäcklund transformations is to yield new solutions of (33) from known solutions; for instance from the trivial solution $u^{(0)}(x,t)=w^{(0)}(x,t)=0$ the single-soliton solution (40) can be readily obtained via (48) and (49) (of course an appropriate time-dependence must be attributed to the x-independent "integration constant" that obtains from the integration of (48), which is an ODE in the independent variable x).

Another important property of Bäcklund transformations is their *commutativity*. Consider two sets of two polynomials, $g^{(m)}(z)$ and $h^{(m)}(z), m=1,2$, and the two Bäcklund transformations (45) they generate, say BT1 and BT2. Take as starting point some function $u^{(0)}(x)$ and associate to it two functions,

$u^{(1)}(x)$ respectively $u^{(2)}(x)$, obtained from $u^{(0)}(x)$ via these two Bäcklund transformations, BT1 respectively BT2. Then obtain a new function, say $u^{(12)}(x)$, from $u^{(1)}(x)$ via BT2; and likewise obtain $u^{(21)}(x)$ from $u^{(2)}(x)$ via BT1. The property of commutativity entails that, provided an appropriate choice is made of integration constants (see (45)),

$$u^{(12)}(x) = u^{(21)}(x) \qquad [50]$$

This property is highly nontrivial when viewed, as we just did, in configuration space; it is instead rather obvious in the spectral space, indeed the corresponding property for the "reflection coefficients" reads (in self-evident notation, see (47b))

$$R^{(12)}(k) = R^{(21)}(k) = R^{(0)}(k)\, B^{(1)}(k)\, B^{(2)}(k) \qquad [51a]$$

$$B^{(m)}(k) = \frac{g^{(m)}(-4\,k^2) + 2ikh^{(m)}(-4\,k^2)}{g^{(m)}(-4\,k^2) - 2ikh^{(m)}(-4\,k^2)}, \quad m = 1,2 \qquad [51b]$$

hence it corresponds simply to the commutativity of the ordinary product.

Nonlinear superposition principle Another remarkable property of the class of evolution equations (33) is a straightforward consequence of the commutativity property, (50), of Bäcklund transformations. It reads (hereafter with a slight abuse of language we refer to "solutions" $w^{(j)}$ even though the actual solutions are the functions $u^{(j)}$ related to the $w^{(j)}$ by (49))

$$w^{(12)} = w^{(21)} = w^{(0)} - \frac{2(p_1 + p_2)\left(w^{(1)} - w^{(2)}\right)}{2(p_1 - p_2) + w^{(1)} - w^{(2)}} \qquad [52]$$

where $w^{(0)} \equiv w^{(0)}(x,t)$ is an arbitrary solution of (33), $w^{(1)} \equiv w^{(1)}(x,t)$ respectively $w^{(2)} \equiv w^{(2)}(x,t)$ are likewise the solutions of the same PDE related to $w^{(0)}$ by the Bäcklund transformation (48) with $p = p_1$ respectively $p = p_2$, and $w^{(12)}(x,t) = w^{(21)}(x,t)$ is another solution of the same PDE. Note that this formula, for which the title of this subsection seems appropriate, provides a completely explicit, rational expression of a new solution of (33) in terms of three other solutions of the same equation: an arbitrary solution $w^{(0)}$, and the two solutions $w^{(1)}$ and $w^{(2)}$ related to it by a simple Bäcklund transformation, see (48).

Soliton ladder A simple application of the preceding formula is to start from the trivial solution

$$w^{(0)} = 0 \qquad [53]$$

so that (see (48))

$$w^{(j)}(x,t) = -2p_j\left[1 - \tan\left\{p_j\left[x - x_0^{(j)} + \alpha(4p^2)t\right]\right\}\right], \quad j = 1,2 \qquad [54a]$$

where, in order that this function be real, either

$$\mathrm{Im}\left[x_0^{(j)}\right] = 0 \qquad [54b]$$

or

$$\mathrm{Im}\left[x_0^{(j)}\right] = \frac{\pi}{2p_j} \qquad [54c]$$

Via (49), the expression (54a) with (54b) yields, for each value of j, a version of the *single-soliton* solution (40). Insertion of (53) and (54a) in (52) yields, via (49), the *two-soliton* solution of (33), provided $0 < p_1 < p_2$ and $x_0^{(1)}$ satisfies (54b) while $x_0^{(2)}$ satisfies (54c) (otherwise the solution produced by (52) is complex or singular).

Having thus obtained the *two-soliton* solution, one can apply the nonlinear superposition formula (52) to get the three-soliton solutions, by inserting in place of $w^{(0)}$ the *single-soliton* expression (54a) (with parameter, say, p_1) and in place of $w^{(1)}$ and $w^{(2)}$ the *two-soliton* expression (with parameters p_1 and p_2 respectively p_1 and p_3); and the process can be continued, as suggested by the title of this subsection. In this manner the multisolitonic solution can be constructed by a sequence of purely algebraic operations: and simple rules can be given, detailing the restrictions on the soliton parameter p_n and the reality properties of the constants $x_0^{(n)}$ ((54b) or (54c)) to insure that the solution so arrived at be real and nonsingular, and thus coincide with (43).

Conservation laws As mentioned above, *integrable* evolution PDEs are interpretable as *infinite-dimensional* dynamical systems. It is therefore natural that they possess an *infinite* number of conserved quantities. For instance every PDE of the class [33] possesses the following infinite sequence of conserved quantities:

$$C_n = \frac{(-1)^n}{2n+1}\int_{-\infty}^{\infty} dx\, \mathbf{R}^n[xu_x(x,t) + 2u(x,t)], \quad n = 0,1,2,\ldots, \qquad [55a]$$

where $\mathbf{R}$ is the recursion operator (34). An alternative definition for this sequence is

$$C_n = \frac{(-1)^n}{2n+1}\int_{-\infty}^{\infty} dx\tilde{\mathbf{R}}^n u(x,t), \quad n = 0,1,2,\ldots, \qquad [55b]$$

where the integrodifferential operator $\tilde{\mathbf{R}}$ is in some sense the adjoint of $\mathbf{R}$, being defined by the formula

$$\tilde{\mathbf{R}}f(x,t) = f_{xx}(x,t) - 4u(x,t)f(x,t) + 2\int_x^{\infty} dy\, u(y,t)f_y(y,t) \qquad [55c]$$

that specifies its action on a generic function $f(x,t)$ (such that the integration converge). The first 3 of these conserved quantities read as follows:

$$C_0 = \int_{-\infty}^{\infty} dx\, u(x,t),$$
$$C_1 = \int_{-\infty}^{\infty} dx\, u^2(x,t),$$
$$C_2 = \int_{-\infty}^{\infty} dx\, [2u^3(x,t) + u_x^2(x,t)]$$

These constants of the motion (55) are functionally independent and, in the context of a Hamiltonian formulation characterized by the Poisson bracket

$$\{A,B\} = \int_{-\infty}^{\infty} dx \frac{\delta A}{\delta u(x)} \frac{\partial}{\partial x} \frac{\delta B}{\delta u(x)}$$

(where A and B are functionals of $u(x)$ and $\delta/\delta u(x)$ denotes the functional derivative), they are *in involution*,

$$\{C_n, C_m\} = 0$$

Note that, in this context, the KdV PDE (35) coincides with the Hamiltonian equation

$$u_t(x,t) = \{u(x,t), H\} = \left(\frac{\partial}{\partial x}\right) \frac{\delta H}{\delta u(x,t)}$$

with

$$H = \frac{1}{2}C_2 = \frac{1}{2}\int_{-\infty}^{\infty} dx\, [2u^3(x,t) + u_x^2(x,t)]$$

Several alternative sequences of constants of motion also exist. For instance another infinite sequence is provided by the two equivalent formulas

$$c_n = (-1)^n \int_{-\infty}^{\infty} dx\, \hat{\mathbf{R}}^{2n} \cdot 1 \qquad [56a]$$

$$c_n = (-1)^n \int_{-\infty}^{\infty} dx\, \Lambda_0^n\, u(x,t) \qquad [56b]$$

with the integrodifferential operators $\hat{\mathbf{R}}$ and Λ_0 defined by the formulas

$$\hat{\mathbf{R}}f(x,t) = f_x(x,t) - \int_{-\infty}^{x} dy\, u(y,t) f(y,t),$$
$$\Lambda_0 f(x,t) = f_{xx}(x,t) - 2u(x,t)f(x,t) + u_x(x,t)\int_x^{\infty} dy\, f(y,t) + u(x,t)\int_x^{\infty} dy\, u(y,t) \int_y^{\infty} dz\, f(z,t)$$

Note that the integrodifferential operator Λ_0 is just Λ, see (46), with $u^{(0)}(x,t) = 0$ and $u^{(1)}(x,t) = u(x,t)$.

The constants c_n are also all independent of each other, but there is a relationship between the constants of the two sequences, (55) and (56),

$$\sum_{n=0} c_n z^{2n+1} = \sin\left[\sum_{n=0} C_n z^{2n+1}\right]$$

which is to be understood by expanding the right-hand side in powers of z and then equating the coefficients of equal powers of z:

$$c_0 = C_0,$$
$$c_1 = C_1 - \tfrac{1}{6}C_0^3,$$
$$c_2 = C2 - \tfrac{1}{2}C_0^2 C_1 + \tfrac{1}{120}C_0^5$$

and so on.

Of course all these conservation laws are applicable to the class of solutions of (33) defined for all (*real*) values of x and vanishing asymptotically (as $x \to \pm\infty$). But they can also be reformulated as *local* "continuity equations". And – rather remarkably – all these results hold as well for the explicitly time-dependent class of PDEs that obtains if one allows the polynomial $\alpha(z)$ in the right-hand side of (33) to feature an *arbitrary* time-dependence, say

$$\alpha(z,t) = \sum_{m=0}^{M} \alpha_m(t) z^m \qquad [57]$$

Finally let us note that there is an additional conserved quantity for this (generalized) class of PDEs,

$$C = \int_{-\infty}^{\infty} dx \left[xu(x,t) + \int_0^t dt' \alpha(\tilde{\mathbf{R}}, t') u(x,t)\right]$$

with $\tilde{\mathbf{R}}$ defined by (55c). This implies that, for the generic solution of this (generalized) class of PDEs the *center of mass*

$$X(t) = \frac{\int_{-\infty}^{\infty} dx\, x\, u(x,t)}{\int_{-\infty}^{\infty} dx\, u(x,t)}$$

moves according to the formula

$$X(t) = X_0 + \sum_{m=0}^{M} (-1)^{m+1} (2m+1) \left(\frac{C_m}{C_0} \right) \times \int_0^t dt' \alpha_m(t'), X_0 = \frac{C}{C_0}$$

Hence for all the *autonomous* evolution PDEs of the class (33) (with $\alpha(z,t) = \alpha(z), \alpha_m(t) = \alpha_m$, see (57)) the center of mass of the *generic* solution moves uniformly,

$$X(t) = X_0 + Vt$$

with the (constant) speed

$$V = \sum_{m=0}^{M} (-1)^{m+1} (2m+1) \left(\frac{C_m}{C_0} \right) \alpha_m$$

Other techniques to identify, classify and investigate integrable PDEs

The spectral transform approach on which we focussed above is just one of the various techniques used to identify and investigate *integrable* nonlinear evolution PDEs. (Incidentally; because the less standard aspect of this approach is the *inverse* transformation to reconstruct, in the framework of the spectral problem, the "potential" $u(x)$ from its spectral transform, this approach is often called the Inverse Spectral, or Scattering, Transform method – abbreviated as IST). In this subsection we tersely mention some other approaches, referring to the literature indicated below for more adequate treatments.

An approach starts from a trivially integrable PDE – say, linear and autonomous, see for instance (30) – and performs a nonlinear change of dependent, and possibly as well of independent, variables. The PDE thus obtained is generally *integrable*, indeed the term *C-integrable* is used to denote such equations (to distinguish them from the *S-integrable* equations solvable via IST: the letter C refers to the Change of variables, the letter S to the Spectral, or Scattering, transform). A simple instance of *C-integrable* equations is the Burgers equation (5), which is linearized via the change of dependent variable

$$\tilde{q}(x,t) = q(x,t) \exp\left[-\int_{-\infty}^{x} dy q(y,t) \right]$$

$$q(x,t) = \frac{\tilde{q}(x,t)}{1 - \int_{-\infty}^{x} dy\, \tilde{q}(y,t)}$$

entailing the linear PDE

$$\tilde{q}_t + \tilde{q}_{xx} = 0$$

A second example is the "Liouville equation"

$$u_{xt} = \exp(u) \qquad [58a]$$

or equivalently, in "light-cone coordinates" ($\xi = x + t$, $\tau = -x + t$)

$$u_{\tau\tau} - u_{\xi\xi} = \exp(u) \qquad [58b]$$

the general solution of which reads

$$u(x,t) = f(x) - g(t) - 2 \log \left\{ a \int_{x_0}^{x} dx' \exp[f(x')] + (2a)^{-1} \int_{t_0}^{t} dt' \exp[-g(t')] \right\}$$

with $f(x)$ and $g(t)$ arbitrary functions and x_0, t_0, a arbitrary constants. And a third example is the Eckhaus equation

$$q_t = i\left\{ q_{xx} + \left[2\left(|q|^2 \right)_x + |q|^4 \right] q \right\} \qquad [59]$$

which is linearized by the transformation

$$\hat{q}(x,t) = q(x,t) \exp\left[\int_{-\infty}^{x} dy |q(y,t)|^2 \right]$$

$$q(x,t) = \frac{\hat{q}(x,t)}{\sqrt{1 + 2\int_{-\infty}^{x} dy |\hat{q}(y,t)|^2}}$$

entailing the linear PDE

$$\hat{q}_t = i\hat{q}_{xx}$$

Thanks to the simplicity of the technique to solve them, *C-integrable* PDEs provide a convenient tool to investigate the phenomenology associated with *nonlinear* PDEs. For instance the Burgers equation (5), which possesses kink-like solitons, is a simple nonlinear generalization of the heat equation; and the "relativistic invariance" of the Liouville equation, see (58b), makes it a convenient "toy model" in the context of relativistic field theory. The Eckhaus equation, (59), provides an interesting theoretical tool because of its similarity with the phenomenologically important NLS equation (6), as well as the fact that, thanks to its *C-integrability*, the structure of its solutions – which feature a remarkable solitonic zoology, including the possibility of "anelastic" solitonic reactions – can be studied in considerable detail, entailing an understanding of why such anelastic reactions are unlikely to be featured by solutions obtained in the context of the initial-value problem.

C-integrable PDEs are generally as well *S-integrable*, being generally associable with a spectral problem that can be explicitly solved; the converse, instead, is not generally true. Hence *C-integrability* represents a higher level of integrability than *S-integrability*; a ranking that is quite useful in spite of its lack of strict cogency caused by the possibility to consider also the transformation from a function to its spectral transform as a change of (dependent) variable.

The Lax approach, described in some detail above in the context of finite-dimensional integrable dynamical systems, was in fact originally invented in the context of integrable PDEs. For instance the KdV equation (35) corresponds to the (operator) Lax equation (to be compared with the matrix Lax equation (14))

$$\mathbf{L}_t = [\mathbf{L}, \mathbf{M}]$$

where now the Schrödinger operator $\mathbf{L}$ is defined by (36) (so that $\mathbf{L}_t = u_t(x,t)$) and the operator $\mathbf{M}$ is defined as follows:

$$\mathbf{M} = -4\left(\frac{\partial}{\partial x}\right)^3 + 6u(x,t)\frac{\partial}{\partial x} + 3u_x(x,t)$$

Closely connected with this approach is the AKNS method (due to M. J. Ablowitz, D. J. Kaup, A. C. Newell and H. Segur), based on the observation that the KdV equation (35) coincides with the integrability condition

$$\psi_{xxt} = \psi_{txx} \qquad [60]$$

for the following pair of linear PDEs (the first of which is just the eigenvalue equation for the Schrödinger operator $\mathbf{L}$, see (36)) satisfied by the function $\psi(x,k,t)$:

$$\psi_{xx} = \left[u(x,t) - k^2\right]\psi \qquad [61a]$$

$$\psi_t = \left[-u_x(x,t) + 4ik^3\right]\psi + 2\left[u(x,t) + 2k^2\right]\psi_x \qquad [61b]$$

and, more generally, that every equation of the class (33) coincides with the integrability condition (60) for the eigenvalue equation (61a) and the equation

$$\psi_t = a(x,k,t)\,\psi + b(x,k,t)\,\psi_x \qquad [61c]$$

with an appropriate choice of the two functions $a(x,k,t)$ and $b(x,k,t)$. Indeed this *ansatz*, (61c), with $a(x,k,t)$ and $b(x,k,t)$ low-order polynomials in k, provides a quite straightforward technique to identify the simpler equations of the class (33); ditto for the extension of this approach based on more general eigenvalue problems than (61a).

Another powerful approach suitable to identify and investigate *integrable* PDEs is the so-called "dressing method" (introduced by V. E. Zakharov and A. B. Shabat and pursued by many others), in which one starts again (as in the approach leading to *C-integrable* equations) from an easily solvable evolution equation and then performs transformations (less elementary than just a change of variables) that modify ("dress") the original equation, obtaining thereby new (nontrivial and interesting) evolution equations, the *integrability* of which hinges on the control one has on the (dressing) transformation relating (both ways) the solutions of the new equations with those of the original equation. Of course many specific techniques are accommodated within this (admittedly vague) description; we must confine our remarks here to noting the crucial role that the Riemann-Hilbert problem generally plays in this context (indeed the Riemann-Hilbert problem also lies at the core of the solvability of the inverse spectral problem, although techniques not explicitly relying on it are also available).

Algorithmic approaches, particularly suitable to manufacture multisolitonic solutions and to identify nonlinear PDEs that are *integrable* inasmuch as they feature such solutions, were developed already at the beginning of the 70's. The pioneer of this approach was R. Hirota; less than a decade later a more sophisticated and general development – the so-called "tau-function" method – was invented by M. Sato and his pupils/collaborators.

Finally let us mention that many remarkable connections exist among *integrable* PDEs and *integrable* finite-dimensional dynamical systems such as those discussed above; for instance the time-evolution (taking generally place in the complex plane) of the poles of *rational* solutions of certain *integrable* PDEs obey the equations of motion of *integrable* dynamical systems interpretable as many-body problems.

Why are certain nonlinear PDEs both integrable and widely applicable?

Several integrable PDEs play a key role in various applicative contexts, justifying the question figuring as title of this subsection. A metamathematical but enlightening, and heuristically quite useful, reply to this question reads as follows.

Consider as starting point a *large* class of nonlinear PDEs, and associate to it via some kind of asymptotic limit procedure a *single* nonlinear

PDE – to which it is then justified to attribute a certain *universal* character. If this procedure corresponds to a *physically* (or, more generally, *applicatively*) significant limit, it stands to reason that this universal PDE play a role in *several* applicative contexts (because the original class of PDEs, being *large*, certainly contains *several* equations of applicative relevance). And if the limit procedure is in some sense *asymptotically exact*, and it therefore *preserves* the property of *integrability*, it is also likely that this universal PDE be *integrable*, because for this it is sufficient that the original, *large* class of PDEs contain just one *integrable* PDE.

For instance most phenomena characterized by a dominant dispersive plane wave in a weakly nonlinear context can be shown, via an asymptotically exact multiscale expansion, to be modeled by the Nonlinear Schroedinger equation (6), the solution of which provides then the evolution, in appropriately rescaled "slow" and "coarse-grained" time and space variables, of the amplitude modulation of the dominant dispersive wave. This explains why this nonlinear PDE plays a key role in so many, disparate applicative contexts, and it also implies, in the light of the above argument, its integrability.

The reasoning outlined above is quite robust, and it allows to infer that, if instead the universal limit equation is *not* integrable, then the large class of PDEs from which it originates cannot contain *any* integrable equation, providing thereby the point of departure to obtain (quite useful) *necessary conditions for integrability*. Indeed these conditions are adequate to distinguish among different levels of integrability, for instance among *C-integrability* and *S-integrability*; with the Eckhaus equation (59) playing in this context a somewhat analogous role for *C-integrable* PDEs to that played by the Nonlinear Schrödinger equation (6) for *S-integrable* PDEs.

Outlook

Many more important developments than could be covered in this overview have occurred in the last few decades; for these we refer to the books listed below (and there are many more), and to the literature cited there.

Let us end this entry by emphasizing that both the study of *integrable systems*, and its application to phenomenologically interesting situation – including technological innovations, for instance in nonlinear optics and telecommunications – are still in the forefront of current research; although perhaps the "heroic era" of this field of study is over.

See also: Abelian Higgs Vortices; Bäcklund Transformations; Bethe Ansatz; Bifurcations of Periodic Orbits; Bi-Hamiltonian Methods in Soliton Theory; Billiards in Bounded Convex Domains; Boundary-Value Problems for Integrable Equations; Breaking Water Waves; Calogero–Moser–Sutherland Systems of Nonrelativistic and Relativistic Type; Cauchy Problem for Burgers-type Equations; Cellular Automata; Classical *r*-Matrices, Lie Bialgebras, and Poisson Lie Groups; $\bar{\partial}$-Approach to Integrable Systems; Einstein Equations: Exact Solutions; Functional Equations and Integrable Systems; Ginzburg–Landau Equation; Hamiltonian Systems: Obstructions to Integrability; Holonomic Quantum Fields; Instantons: Topological Aspects; Integrability and Quantum Field theory; Integrable Discrete Systems; Integrable Systems and Algebraic Geometry; Integrable Systems and Discrete Geometry; Integrable Systems and the Inverse Scattering Method; Integrable Systems in Random Matrix Theory; Inverse Problem in Classical Mechanics; Isochronous Systems; Isomonodromic Deformations; Integrable Systems and Recursion Operators on Symplectic and Jacobi Manifolds; Korteweg–de Vries Equation and Other Modulation Equations; Multi-Hamiltonian Systems; Nonlinear Schrödinger Equations; Ordinary Special Functions; Painlevé Equations; Peakons; *q*-Special Functions; Quantum Calogero–Moser Systems; Quantum *n*-Body Problem; Random Matrix Theory in Physics; Recursion Operators in Classical Mechanics; Riemann–Hilbert Methods in Integrable Systems; Riemann–Hilbert Problem; Separation of Variables for Differential Equations; Sine-Gordon Equation; Solitons and Kac–Moody Lie Algebras; Solitons and Other Extended Field Configurations; Twistors; Toda Lattices; Vortex Dynamics; WDVV Equations and Frobenius Manifolds; Yang–Baxter Equations.

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Interacting Particle Systems and Hydrodynamic Equations

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Introduction

We present the theory of hydrodynamic behavior of interacting particle systems in the context of exclusion processes, in which no more than one particle per site is allowed.

Denote by $\mathbb{T}_N = \mathbb{Z}/N\mathbb{Z}$ the discrete torus with N points and let $\mathbb{T}_N^d = (\mathbb{T}_N)^d$. The state space $\mathcal{E}_N = \{0,1\}^{\mathbb{T}_N^d}$ consists of all configurations obtained by distributing particles on the discrete torus $\mathbb{T}_N^d$ respecting the exclusion rule which prevents more than one particle per site. The configurations are denoted by the Greek letter η so that $\eta(x)$ is equal to 0 or 1 if site $x \in \mathbb{T}_N^d$ is vacant or occupied for the configuration η.

Denote by $\{\tau_x : x \in \mathbb{Z}^d\}$ the group of translations in $\mathcal{E}_N$: $(\tau_x\eta)(z) = \eta(x+z)$ for each x, z in $\mathbb{Z}^d$. Here and below summations are performed modulo N. A function $f : \{0,1\}^{\mathbb{Z}^d} \to \mathbb{R}$ with finite support is called a cylinder function.

Fix a family of non-negative cylinder functions c_j, $1 \le j \le d$. Let $c_{x,x+e_j}(\eta) = c_j(\tau_x\eta)$ and consider the Markov process $\{\eta_t : t \ge 0\}$ on $\mathcal{E}_N$ with generator L_N given by

$$(L_N f)(\eta) = \sum_{j=1}^{d} \sum_{x \in \mathbb{T}_N^d} c_{x,x+e_j}(\eta)[f(\sigma^{x,x+e_j}\eta) - f(\eta)] \quad [1]$$

Here, $\{e_1, \ldots, e_d\}$ stands for the canonical basis of $\mathbb{R}^d$ and $\sigma^{x,y}\eta$ for the configuration obtained from η by exchanging the occupation variables $\eta(x)$ and $\eta(y)$:

$$(\sigma^{x,y}\eta)(z) = \begin{cases} \eta(z) & \text{if } z \ne x, y \\ \eta(y) & \text{if } z = x \\ \eta(x) & \text{if } z = y \end{cases} \quad [2]$$

In this dynamics at each bond $\{x, x+e_j\}$ the occupation variables $\eta(x), \eta(x+e_j)$ are exchanged at rate $c_{x,x+e_j}(\eta)$. This happens simultaneously and independently at each bond.

Notice that the total number of particles is conserved by the dynamics since only exchanges are allowed. Denote by $\Sigma_{N,K}(0 \le K \le |\mathbb{T}_N^d|)$ the hyperplane of all configurations η of $\mathcal{E}_N$ with K particles. Assume that the rates c_j are nondegenerate for η_t to be an irreducible Markov process on each $\Sigma_{N,K}$.

For $0 \le \alpha \le 1$, denote by ν_α^N the Bernoulli product measure of parameter α on $\mathcal{E}_N$. Under ν_α^N, the variables $\{\eta(x), x \in \mathbb{T}_N^d\}$ are independent, with marginals given by

$$\nu_\alpha^N\{\eta(x) = 1\} = \alpha = 1 - \nu_\alpha^N\{\eta(x) = 0\}$$

Assume that the measures $\nu_\alpha^N, 0 \le \alpha \le 1$ are stationary for the Markov process η_t. An elementary computation shows that this is the case if each function c_j does not depend on $\eta(0)$, $\eta(e_j)$, in which case the process is in fact reversible with respect to ν_α^N.

Let $\mathcal{M}_+(\mathbb{T}^d)$ be the space of finite positive measures on the torus $\mathbb{T}^d$ endowed with the weak topology. For each configuration η, let $\pi^N = \pi^N(\eta, \mathrm{d}u)$ be the positive measure on $\mathbb{T}^d$ obtained by assigning mass N^{-d} to each particle:

$$\pi^N := N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x)\delta_{x/N}(\mathrm{d}u) \quad [3]$$

where δ_u stands for the Dirac measure on u. The measure π^N is called the empirical measure associated to the configuration η. The integral of a continuous function $G : \mathbb{T}^d \to \mathbb{R}$ with respect to π^N is denoted by

$$\langle \pi^N, G \rangle = N^{-d} \sum_{x \in \mathbb{T}_N^d} G(x/N)\eta(x)$$

Fix a density profile $\rho_0 : \mathbb{T}^d \to [0,1]$. A sequence of probability measures μ^N on $\mathcal{E}_N$ is said to be associated to ρ_0 if π^N converges in probability to $\rho_0(u)\mathrm{d}u$ under μ^N:

$$\lim_{N\to\infty} \mu^N \left\{ \left| \langle \pi^N, G \rangle - \int_{\mathbb{T}^d} G(u)\rho_0(u)\,\mathrm{d}u \right| > \delta \right\} = 0$$

for all continuous functions $G:\mathbb{T}^d \to \mathbb{R}$ and all $\delta > 0$. For a continuous profile ρ_0 consider, for instance, the product measure $\nu^N_{\rho_0(\cdot)}$ on $\mathcal{E}_N$ whose marginals are given by

$$\nu^N_{\rho_0(\cdot)}\{\eta(x) = 1\} = \rho_0(x/N)$$

It is easy to check that the sequence of probability measures $\nu^N_{\rho_0(\cdot)}$ is associated to ρ_0.

Denote by $W_{x,x+e_j}$ the instantaneous current of particles from x to $x + e_j$. This is the rate at which a particle jumps from x to $x + e_j$ minus the rate at which a particle jumps from $x + e_j$ to x:

$$W_{x,x+e_j} = \{\eta(x) - \eta(x + e_j)\}c_{x,x+e_j}(\eta)$$

Suppose that the mean value of the current vanishes under all stationary states ν^N_α. This denotes that the average displacement of each particle vanishes in the mean. In particular, in view of the central limit theorem, to observe an evolution of the density in the macroscopic scale, a diffusive rescaling of time is needed. On the other hand, if there is a net flux of particles, the evolution has to be examined in the Euler scale tN.

Denote by $\theta(N)$ the time rescaling: N^2 if the mean displacement of particles vanishes and N otherwise. For each probability measure μ^N on $\mathcal{E}_N$, let $\mathbb{P}_{\mu^N}$ be the probability measure on the path space $D(\mathbb{R}_+, \mathcal{E}_N)$ induced by μ^N and the Markov process η_t speeded up by $\theta(N)$. Expectation with respect to $\mathbb{P}_{\mu^N}$ is denoted by $\mathbb{E}_{\mu^N}$.

Denote by $\pi^N_t(\mathrm{d}u) = \pi^N(\eta_{t\theta(N)}, \mathrm{d}u)$ the empirical measure at time t. Fix a density profile $\rho_0:\mathbb{T}^d \to [0,1]$ and a sequence of probability measures μ^N on $\mathcal{E}_N$ associated to ρ_0. The goal of the theory of hydrodynamic limit of interacting particle systems is to show that for each $t > 0, \pi^N_t$ converges, as $N \uparrow \infty$, to a deterministic path $\pi(t, \mathrm{d}u) = \rho(t, u)\mathrm{d}u$ whose density ρ is the solution of some partial differential equation, called the hydrodynamic equation.

The main tools available are entropy production and Dirichlet forms. Denote by $H_N(\mu^N|\nu^N)$ the entropy of a probability measure μ^N on $\mathcal{E}_N$ with respect to a reference probability measure ν^N:

$$H_N(\mu^N|\nu^N) = \sup_f \left\{ \int_{\mathcal{E}_N} f\,\mathrm{d}\mu^N - \log \int_{\mathcal{E}_N} \mathrm{e}^f\,\mathrm{d}\nu^N \right\}$$

where the supremum is carried over all functions $f:\mathcal{E}_N \to \mathbb{R}$.

It follows from the general theory of Markov processes that the entropy of the state of the process with respect to an invariant state decreases in time. The rate at which the entropy production decreases can be estimated by the Dirichlet form: let S^N_t be the semigroup associated to the generator L_N defined in [1] speeded up by $\theta(N)$. An elementary computation gives that

$$\begin{aligned} &H_N(\mu^N S^N_t|\nu^N_\alpha) + 2\theta(N)\int_0^t \mathrm{d}s\, I^N_\alpha(\mu^N S^N_s) \\ &\quad \le H_N(\mu^N|\nu^N_\alpha) \end{aligned}$$

Here, $I^N_\alpha(\mu^N)$ is the convex and lower semicontinuous functional given by

$$I^N_\alpha(\mu^N) = -\langle f^{1/2}, L_N f^{1/2}\rangle_{\nu^N_\alpha}$$

where f stands for the Radon–Nikodym derivative $\mathrm{d}\mu^N/\mathrm{d}\nu^N_\alpha$ and $\langle\cdot,\cdot\rangle_{\nu^N_\alpha}$ for the scalar product in $L^2(\nu^N_\alpha)$.

Therefore, if the initial state μ^N has entropy with respect to a reference measure ν^N_α bounded by C_0N^d, by convexity of I^N_α,

$$\begin{aligned} &N^{-d}H_N(\mu^N S^N_t|\nu^N_\alpha) \\ &\quad + 2t\theta(N)N^{-d}I^N_\alpha\left(t^{-1}\int_0^t \mathrm{d}s\mu^N S^N_s\right) \le C_0 \end{aligned} \qquad [4]$$

for all $t \ge 0$. This elementary estimate plays a fundamental role in the following sections.

The Entropy Method

Consider an exclusion process with generator given by [1]. Fix $T > 0$, a density profile $\rho_0:\mathbb{T}^d \to [0,1]$ and a sequence of probability measures μ^N associated to ρ_0. Let $\mathbb{Q}_{\mu^N}$ be the measure on the path space $D([0,T], \mathcal{M}_+(\mathbb{T}^d))$ induced by the process π^N_t and the initial state μ^N.

To prove that π^N_t converges to $\rho(t,u)\mathrm{d}u$ in probability, we first show that the sequence $\mathbb{Q}_{\mu^N}$ converges to the probability measure $\mathbb{Q}^*$ concentrated on the deterministic trajectory $\rho(t,u)\mathrm{d}u$, whose density is the solution of some partial differential equation with initial condition ρ_0. It follows from this result and general arguments that π^N_t converges to $\rho(t,u)\mathrm{d}u$ for each $0 \le t \le T$.

To prove that $\mathbb{Q}_{\mu^N}$ converges to $\mathbb{Q}^*$, assume that we are able to prove tightness of the sequence $\mathbb{Q}_{\mu^N}$. Since there is at most one particle per site, all limit points $\mathbb{Q}^*$ of the sequence $\mathbb{Q}_{\mu^N}$ are concentrated on trajectories $\pi(t,\mathrm{d}u) = \rho(t,u)\mathrm{d}u$, which are absolutely continuous with respect to Lebesgue.

To characterize the limit points $\mathbb{Q}^*$, fix a smooth function $G:\mathbb{T}^d \to \mathbb{R}$ and consider the martingale

$$\begin{aligned} M^{G,N}_t &= \langle \pi^N_t, G\rangle - \langle \pi^N_0, G\rangle \\ &\quad - \int_0^t \theta(N)L_N\langle \pi^N_s, G\rangle\,\mathrm{d}s \end{aligned} \qquad [5]$$

An elementary computation of its quadratic variation shows that $M_t^{G,N}$ vanishes in $L^2(\mathbb{P}_{\mu^N})$ as $N \uparrow \infty$.

Denote by $\mathcal{C}_0$ the space of cylinder functions which have zero mean with respect to all invariant states ν_α^N. Assume that the currents $W_{0,e_j}, 1 \le j \le d$, belong to $\mathcal{C}_0$ so that a diffusive scaling $\theta(N) = N^2$ is in force. Notice that

$$L_N \eta(x) = \sum_{j=1}^{d} W_{x-e_j,x} - W_{x,x+e_j}$$

In particular, after a summation by parts, the integral term on the right-hand side of [5] can be written as

$$\int_0^t N^{1-d} \sum_{j=1}^{d} \sum_{x \in \mathbb{T}_N^d} (\nabla_{u_j}^N H)(x/N) W_{x,x+e_j}(s)\, ds \qquad [6]$$

where $(\nabla_{u_j}^N H)(x/N) = N\{H(x+e_j/N) - H(x/N)\}$. Notice that this sum is in principle of order N.

To illustrate the entropy method, consider the symmetric simple exclusion process obtained by taking $c_j = 1/2$ in [1] and observe that the current $W_{0,e_j} = (1/2)\{\eta(0) - \eta(e_j)\}$. A second summation by parts permits to rewrite the martingale [5] as

$$\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle - \frac{1}{2}\int_0^t \langle \pi_s^N, \Delta_N G\rangle\, ds$$

where Δ_N is the discrete Laplacian.

Since the martingale $M_t^{G,N}$ vanishes in $L^2(\mathbb{P}_{\mu^N})$, as $N \uparrow \infty$, all limit points $\mathbb{Q}^*$ are concentrated on weak solutions of the linear heat equation. It remains to recall that there is a unique weak solution of the Cauchy problem for the heat equation to conclude that the sequence $\mathbb{Q}_{\mu^N}$ converges to $\mathbb{Q}^*$, the measure concentrated on the deterministic path $\pi_t(du) = \rho(t,u)du$ whose density ρ is the solution of the heat equation with initial condition ρ_0.

The symmetric simple exclusion process has the very special property that the martingale $M_t^{G,N}$ can be written as a function of the empirical measure. This is not the case for all the other models, for which a further argument is needed to close eqn [5] in terms of the empirical measure.

To present the additional arguments needed, assume that $c_j(\eta) = 1 + [\eta(-e_j) + \eta(2e_j)]$. In this case, the current W_{0,e_j} is equal to

$$\{\eta(0) - \eta(e_j)\} + \{\eta(0)\eta(-e_j) - \eta(e_j)\eta(2e_j)\} + \{\eta(0)\eta(2e_j) - \eta(-e_j)\eta(e_j)\}$$

A second summation by parts in [6] permits to rewrite it as

$$\int_0^t N^{-d} \sum_{j=1}^{d} \sum_{x \in \mathbb{T}_N^d} (\partial_{u_j}^2 H)(x/N) \tau_x h(\eta_{sN^2})\, ds + o_N(1) \qquad [7]$$

where $h(\eta) = \eta(0) + 2\eta(0)\eta(-e_j) - \eta(0)\eta(2e_j)$. The remainder $o_N(1)$ appears because we replaced discrete space derivatives by continuous ones.

In contrast with the symmetric simple exclusion process, the martingale $M_t^{G,N}$ defined in [5] is not a function of the empirical measure and an argument is needed to close the equation.

For each positive integer ℓ and d-dimensional integer x, denote by $\eta^\ell(x)$ the empirical density of particles in a box of length $2\ell + 1$ centered at x:

$$\eta^\ell(x) = \frac{1}{(2\ell+1)^d} \sum_{|y-x| \le \ell} \eta(y)$$

For a cylinder function $h : \mathcal{E}_N \to \mathbb{R}$, let $\tilde{h}(\alpha)$ be the expected value of h with respect to the invariant state $\nu_\alpha^N : \tilde{h}(\alpha) = E_{\nu_\alpha^N}[h(\eta)]$. For $\ell \ge 1$ and a cylinder function h, let

$$V_\ell(\eta) = \left| \frac{1}{(2\ell+1)^d} \sum_{|y| \le \ell} (\tau_y h)(\eta) - \tilde{h}(\eta^\ell(0)) \right|$$

Theorem 1 *Consider a sequence of probability measures m^N on $\mathcal{E}_N$ such that $I_\alpha^N(m^N) \le C_0 N^{d-2}$ for some $0 < \alpha < 1$ and some finite constant C_0. Then,*

$$\limsup_{\varepsilon \to 0} \limsup_{N \to \infty} \mathbb{E}_{\mu^N} \left[N^{-d} \sum_{x \in \mathbb{T}_N^d} \tau_x V_{\varepsilon N}(\eta) \right] = 0$$

This statement, due to Guo *et al.* (1988), permits the replacement of a local function h by a function of the density of particles over a macroscopic cube. It is the main step in the proof of the hydrodynamic behavior of gradient systems, defined below, and its proof can be found in Kipnis and Landim (1999, chapter 5).

Assume that the sequence μ^N has entropy with respect to a reference invariant state ν_α^N bounded by $C_0 N^d$ for some finite constant C_0. It follows from [4] that the sequence of measures $T^{-1} \int_0^T ds \mu^N S_s^N$ satisfies the assumptions of Theorem 1. Therefore, due to the presence of the time integral, we may replace the cylinder function h in [7] by $\tilde{h}(\eta^{\varepsilon N}(x))$. Since $\eta^{\varepsilon N}(0)$ can be written as $\langle \pi^N, \iota_\varepsilon \rangle$, where $\iota_\varepsilon = (2\varepsilon)^{-d} 1\{[-\varepsilon, \varepsilon]^d\}$, we now have expressed the martingale [5] in terms of the empirical measure.

Repeating the arguments presented for the symmetric simple exclusion process, we may conclude that all limit points $\mathbb{Q}^*$ of the sequence $\mathbb{Q}_{\mu^N}$ are concentrated on paths $\pi_t(du) = \rho(t,u)du$, whose density ρ is a weak solution of the parabolic equation

$$\begin{cases} \partial_t \rho = \Delta(\rho + \rho^2) \\ \rho(0, \cdot) = \rho_0(\cdot) \end{cases}$$

because $\tilde{h}(\alpha) = \alpha + \alpha^2$ for $h(\eta) = \eta(0) + 2\eta(0)\eta(-e_j) - \eta(0)\eta(2e_j)$. It remains to show the uniqueness of weak solutions of this differential equation to conclude.

The second integration by parts in [6] was possible because the currents could be written as the difference of local functions and their translations, a very special property not shared by most interacting particle systems. Processes with this attribute are called gradient systems.

Nongradient Models

Consider an exclusion process with rates $c_j(\eta) = 1 + \eta(-e_j)$, in which case the current is given by

$$W_{0,e_j} = \{\eta(0) - \eta(e_j)\} + \{\eta(0) - \eta(e_j)\}\eta(-e_j)$$

a cylinder function in $\mathcal{C}_0$.

Fix $T > 0$, a density profile $\rho_0 : \mathbb{T}^d \to [0,1]$ and a sequence of probability measures μ^N associated to ρ_0 and having entropy with respect to a reference invariant state ν_α^N bounded by $C_0 N^d$ for some finite constant C_0. Recall the definition of the sequence of measures $\mathbb{Q}_{\mu^N}$, assumed to be tight.

To characterize the limit points of $\mathbb{Q}_{\mu^N}$, fix a smooth function $G : \mathbb{T}^d \to \mathbb{R}$ and examine the martingale $M_t^{G,N}$ introduced in [5]. After an integration by parts, the integral term of the martingale becomes [6]. While a second integration by parts is possible for the first part of the current $\eta(0) - \eta(e_j)$, the second piece remains

$$\int_0^t N^{1-d} \sum_{j=1}^d \sum_{x \in \mathbb{T}_N^d} (\nabla_{u_j}^N H)(x/N) \tau_x w_j(\eta_{sN^2})\, ds \quad [8]$$

where $w_j = \{\eta(0) - \eta(e_j)\}\eta(-e_j)$. Notice the extra factor N multiplying the sum and that w_j belongs to $\mathcal{C}_0$. The next result and Theorem 4 are due to Varadhan (1994).

Theorem 2 *Consider a sequence of probability measures m^N on $\mathcal{E}_N$ such that $H_N(m^N|\nu_\alpha^N) \le C_0 N^d$ for some $0 < \alpha < 1$ and some finite constant C_0. Fix a smooth function $G : \mathbb{T}^d \to \mathbb{R}$ and a cylinder function Ψ in $\mathcal{C}_0$. There exists a seminorm $\|\cdot\|_\alpha$ such that*

$$\limsup_{N\to\infty} \left\{ \mathbb{E}_{m^N} \left[\left| \int_0^T ds N^{1-d} \sum_{x \in \mathbb{T}_N^d} G(x/N) \tau_x \Psi(\eta_{sN^2}) \right| \right] \right\}^2 \le C_0 T \|G\|_2^2 \sup_{0 \le \alpha \le 1} \|\Psi\|_\alpha^2 \quad [9]$$

The explicit form of the seminorm $\|\cdot\|_\alpha$ can be found in Kipnis and Landim (1999, chapter 7). The proof of Theorem 2 requires a sharp estimate on the spectral gap of the generator L_N. Denote by Λ_ℓ the cube $\{-\ell, \ldots, \ell\}^d$ and by L_{Λ_ℓ} the restriction of the generator L_N to the cube Λ_ℓ, obtained by suppressing all jumps from Λ_ℓ (resp. Λ_ℓ^c) to Λ_ℓ^c (resp. Λ_ℓ). For $0 \le K \le |\Lambda_\ell|$, let $\nu_{\Lambda_\ell,K}$ be the uniform measure on the configurations of $\{0,1\}^{\Lambda_\ell}$ with K particles. The following estimate is needed in the proof of Theorem 2:

Theorem 3 *There exists a finite constant C_0 such that*

$$\langle f, f \rangle_{\nu_{\Lambda_\ell,K}} \le C_0 \ell^2 \langle f, (-L_{\Lambda_\ell}) f \rangle_{\nu_{\Lambda_\ell,K}}$$

for all $\ell \ge 1, 0 \le K \le |\Lambda_\ell|$ and zero-mean function f in $L^2(\nu_{\Lambda_\ell,K})$.

This result is due to Quastel (1992) for symmetric simple exclusion processes. Yau developed a general method to prove sharp estimates for the spectral gap of the generator for conservative dynamics (see Lu and Yau (1993) and Yau (1997)).

Since the parallelogram identity is easy to check, by polarization we can define a semi-inner product $\ll \cdot, \cdot \gg_\alpha$ from the seminorm $\|\cdot\|_\alpha$. Denote by $\mathcal{H}_\alpha$ the Hilbert space induced by $\mathcal{C}_0$ and the semi-inner product $\ll \cdot, \cdot \gg_\alpha$.

Denote by L the generator [1] extended to $\mathbb{Z}^d$. Notice that Lf belongs to $\mathcal{C}_0$ for any cylinder function f, and that the gradients $\eta(e_j) - \eta(0)$, and the currents $w_j, 1 \le j \le d$, also belong to $\mathcal{C}_0$. The next result states that all functions in $\mathcal{H}_\alpha$ can be written as a linear combination of gradients and cylinder functions in the image of the generator.

Theorem 4 *Denote by $L\mathcal{C}_0$ the space $\{Lg : g \in \mathcal{C}_0\}$. For each $0 \le \alpha \le 1$,*

$$\mathcal{H}_\alpha = \overline{L\mathcal{C}_0} \oplus \{\eta(e_j) - \eta(0) : 1 \le j \le d\}$$

In particular, there exists a matrix $\{D_{i,j}(\alpha) : 1 \le i, j \le d\}$ and a sequence of functions $\{f_{i,k}(\alpha, \cdot) \in \mathcal{C}_0 : k \ge 1\}, 1 \le i \le d$, for which

$$w_i + \sum_{j=1}^d D_{i,j}(\alpha)\{\eta(e_j) - \eta(0)\} - Lf_{i,k}(\alpha, \cdot)$$

vanishes in $\mathcal{H}_\alpha$ as $k \uparrow \infty$. For reversible systems (and more generally for generators satisfying a sector condition), it can be shown that the sequence of local functions $f_{i,k}(\alpha, \eta)$ can be taken independent of α: $f_{i,k}(\alpha, \eta) = f_{i,k}(\eta)$. Moreover, with a little extra effort, one obtains a bound uniform in α:

$$\inf_{f \in \mathcal{C}_0} \sup_{0 \le \alpha \le 1} \left\| w_i + \sum_{j=1}^d D_{i,j}(\alpha)\{\eta(e_j) - \eta(0)\} - Lf \right\|_\alpha = 0 \quad [10]$$

This estimate together with some algebraic relations in $\mathcal{H}_\alpha$ give a variational formula for the matrix $D_{i,j}$:

for every vector v in $\mathbb{R}^d$,

$$v \cdot D(\alpha)v = \frac{1}{\alpha(1-\alpha)} \inf_{f \in \mathcal{C}_0} \left\| \sum_{i=1}^{d} v_i w_i - Lf \right\|_\alpha^2 \qquad [11]$$

It can also be shown that the matrix D is continuous and strictly elliptic.

We may now complete the proof of the hydrodynamic behavior. Recall that the main difficulty was to express formula [8] in terms of the empirical measure. Fix $1 \le i \le d$ and consider a sequence of cylinder functions $\{f_{i,k} : k \ge 1\}$ satisfying [10] asymptotically as $k \uparrow \infty$. Adding and subtracting the expression $\sum_{1 \le k \le d} D_{j,k}(\eta^{\varepsilon N}(0))\{\eta^{\varepsilon N}(e_j) - \eta^{\varepsilon N}(0)\} - Lf_{j,k}$, [8] becomes the sum of three terms.

The first one is just the expression which appears inside the expectation in [9] with $G = (\nabla^N_{u_j} H)$ and Ψ given by

$$w_j + \sum_{k=1}^{d} D_{j,k}(\eta^{\varepsilon N}(0))\{\eta^{\varepsilon N}(e_j) - \eta^{\varepsilon N}(0)\} - Lf_{j,k}$$

Since the sequence of measure μ^N satisfies the assumptions of Theorem 2, a modification of the proof of this theorem, to take into account the dependence of Ψ on N and ε, shows that the limit of the expectation of the absolute value of the first term in the decomposition, as $N \uparrow \infty$ and then $\varepsilon \downarrow 0$, is bounded by

$$C_0 T \|\partial_{u_j} H\|_2^2 \sup_{0 \le \alpha \le 1} \|\Psi_{j,\alpha}\|_\alpha^2$$

where

$$\Psi_{j,\alpha} = w_j + \sum_{k=1}^{d} D_{j,k}(\alpha)\{\eta(e_j) - \eta(0)\} - Lf_{j,k}$$

By [10], the penultimate expression vanishes as $k \uparrow \infty$.

The second term in the decomposition is

$$\int_0^t \mathrm{d}s N^{1-d} \sum_{j,k=1}^{d} \sum_{x \in \mathbb{T}^d_N} (\nabla^N_{u_j} H)(x/N) \tau_x L f_{j,k}(\eta_{sN^2})$$

The presence of the generator L and the diffusive rescaling of time permit to show that the expectation of the absolute value of this expression is of order N^{-1} for each fixed k.

Finally, the third term is equal to

$$-\int_0^t \mathrm{d}s N^{1-d} \sum_{j,k=1}^{d} \sum_{x \in \mathbb{T}^d_N} (\nabla^N_{u_j} H)(x/N) D_{j,k} \times \left(\eta^{\varepsilon N}_{sN^2}(x)\right)\left\{\eta^{\varepsilon N}_{sN^2}(x+e_k) - \eta^{\varepsilon N}_{sN^2}(x)\right\}$$

A second integration by parts is now possible and one obtains that the previous expression is equal to

$$\int_0^t \mathrm{d}s N^{-d} \sum_{j,k=1}^{d} \sum_{x \in \mathbb{T}^d_N} (\partial^2_{u_j,u_k} H)(x/N)\, d_{j,k}\left(\eta^{\varepsilon N}_{sN^2}(x)\right) + o_N(1)$$

where $d'_{j,k} = D_{j,k}$. We have already seen in the derivation of the hydrodynamic equation for gradient systems that this sum can be expressed as a function of the empirical measure. Since all limit points are concentrated on paths $\pi_t(\mathrm{d}u)$ which are absolutely continuous, this integral converges to

$$\sum_{j,k=1}^{d} \int_0^t \mathrm{d}s \int_{\mathbb{T}^d} \mathrm{d}u (\partial^2_{u_j,u_k} H)(u)\, \mathrm{d}_{j,k}(\rho(s,u))$$

Since the martingale [5] vanishes, all limit points are concentrated on trajectories $\pi_t(\mathrm{d}u) = \rho(t,u)\mathrm{d}u$ which are weak solutions of

$$\partial_t \rho = \sum_{j,k=1}^{d} \partial_{u_j}\left\{\left[\delta_{j,k} + D_{j,k}(\rho)\right]\partial_{u_k}\rho\right\}$$

where D is the strictly elliptic and continuous matrix given by the variational formula [11]. Here, the identity matrix $\delta_{j,k}$ comes from the first piece of the current which permitted a second integration by parts. A uniqueness result of weak solutions of the Cauchy problem with initial condition ρ_0 concludes the proof of the hydrodynamic behavior of this nongradient system.

Hyperbolic Equations

Consider the asymmetric simple exclusion process obtained by setting $c_j(\eta) = \eta(0)[1 - \eta(e_j)]$ in formula [1]. Notice that the current $W_{0,e_j} = \eta(0)[1 - \eta(e_j)]$ has mean $\alpha(1-\alpha)$ with respect to the invariant state ν^N_α, suggesting the Euler rescaling of time $\theta(N) = N$.

Let $\le$ be the partial order on $\mathcal{E}_N$ defined by $\eta \le \xi$ if $\eta(x) \le \xi(x)$ for every x in $\mathbb{T}^d_N$. The asymmetric exclusion process is attractive: there exists a stochastic evolution on $\mathcal{E}_N \times \mathcal{E}_N$ with the following two properties: (1) it preserves the order, in the sense that $\eta_t \le \xi_t$ for all $t \ge 0$ if $\eta_0 \le \xi_0$ and (2) each coordinate evolves according to the original asymmetric exclusion dynamics. This coupling, which may be constructed by letting particles jump together as much as possible, is the main tool in the derivation of the hydrodynamic equation of asymmetric processes.

Fix a smooth function $G : \mathbb{T}^d \to \mathbb{R}$ and recall definition [5] of the martingale $M^{G,N}_t$. An elementary computation shows that the quadratic variation of this martingale vanishes as $N \uparrow \infty$. On the other

hand, after an integration by parts, the integral term of the martingale becomes

$$\int_0^t N^{-d} \sum_{j=1}^{d} \sum_{x \in \mathbb{T}_N^d} (\nabla_{u_j}^N H)(x/N)\eta_{sN}(x) \times [1 - \eta_{sN}(x + e_j)]\, ds$$

Assume that the state of the process at any macroscopic time s is close to a product measure associated to some profile $\rho(s,\cdot)$. Since the martingale vanishes asymptotically, taking expectations in [5], we obtain that the density profile should be a weak solution of the quasilinear hyperbolic equation

$$\partial_t \rho + \sum_{j=1}^{d} \partial_{u_j} F(\rho) = 0 \qquad [12]$$

where $F(a) = a(1 - a)$.

It is well known that solutions of this equation may develop shocks even if the initial profile $\rho_0(\cdot)$ is smooth and that there is no uniqueness of weak solutions. Several criteria have been introduced to select the relevant solution among the weak solutions. Kružkov (1970), for instance, in the case where density profile $\rho_0 : \mathbb{T}^d \to \mathbb{R}$ is bounded, proved that there exists a unique measurable function ρ which satisfies the entropy condition

$$\partial_t |\rho - c| + \sum_{i=1}^{d} \partial_{u_i} |F(\rho) - F(c)| \leq 0 \qquad [13]$$

in the sense of distributions on $(0,\infty) \times \mathbb{T}^d$, for every $c \in \mathbb{R}$, and which converges to the initial condition in $L^1(\mathbb{T}^d)$ as $t \downarrow 0$: $\lim_{t\to 0} \|\rho_t - \rho_0\|_1 = 0$.

Fix $T > 0$ and a density profile $\rho_0 : \mathbb{T}^d \to [0,1]$. To couple the original process with another one starting from a different initial sate, we need to impose the initial distribution to be of product form. Consider, therefore, a sequence of "product" probability measures μ^N associated to ρ_0 and recall the definition of the sequence of measures $\mathbb{Q}_{\mu^N}$ given in the section "The entropy method," assumed to be tight.

We have to prove that all limit points are concentrated on entropy solutions of [12]. Coupling the original process η_t with another one, denoted by ξ_t, starting from the Bernoulli product measure with density α, and examining the time evolution of $\sum_{x\in\mathbb{T}_N^d} |\eta_{tN}(x) - \xi_{tN}(x)|$, we derive an entropy inequality at the microscopic level: let $\bar{\mu}^N$ be a sequence of probability measures on the product space $\mathcal{E}_N \times \mathcal{E}_N$ whose first coordinate is μ^N. Denote by $\mathbb{P}_{\bar{\mu}^N}^N$ the measure on the path space $D([0,T], \mathcal{E}_N \times \mathcal{E}_N)$ induced by $\bar{\mu}^N$ and the coupling informally described at the beginning of this section. Rezakhanlou (1991) proved the following theorem:

Theorem 5 *For every smooth positive function H with compact support in $(0,\infty) \times \mathbb{T}^d$ and every $\varepsilon > 0$,*

$$\lim_{\ell\to\infty} \lim_{N\to\infty} \mathbb{P}_{\bar{\mu}^N}^N \left[\int_0^\infty dt\, N^{-d} \sum_{x\in\mathbb{T}_N^d} \left\{ \partial_t H(t,x/N) |\eta_t^\ell(x) - \xi_t^\ell(x)| + \sum_{i=1}^{d} (\partial_{u_i} H)(t,x/N) |F(\eta_t^\ell(x)) - F(\xi_t^\ell(x))| \right\} \geq -\varepsilon \right] = 1$$

If we now assume that the second coordinate ξ_t is initially distributed according to the stationary state ν_α^N, it is not difficult to replace ξ_t^ℓ in the above formula by α, obtaining a microscopic version of the entropy inequality.

In the one-dimensional nearest-neighbor case, by coupling arguments, we may replace the average $\eta^\ell(0)$ over a large microscopic box by an average $\eta^{\varepsilon N}(0)$ over a small macroscopic box, deriving the entropy inequality [13]. To conclude the proof it remains to show, by means of coupling argument again, that the density profile at time t converges in $L^1(\mathbb{T}^d)$ to the initial condition as $t \downarrow 0$.

In higher dimensions or in the one-dimensional non-nearest-neighbor case, it has not been proved that replacement of $\eta^\ell(0)$ by $\eta^{\varepsilon N}(0)$ is allowed. One is thus forced to consider measure-valued solutions of eqn [12]. Details can be found in Kipnis and Landim (1999, chapter 8).

Relative Entropy Method

The relative entropy method, due to Yau (1991), is based on the analysis of the time evolution of the entropy of the state of the process with respect to the product measure associated to the solution of the hydrodynamic equation.

While the entropy method requires uniqueness of weak solutions and proves the existence of weak solutions, the relative entropy method requires the existence of a smooth solution and proves the uniqueness of such smooth solutions.

Consider the exclusion process with rates $c_j(\eta) = 1 + [\eta(-e_j) + \eta(2e_j)]$. We have seen that the hydrodynamic equation of this model is given by the nonlinear parabolic equation

$$\partial_t \rho = \Delta\{\rho + \rho^2\} \qquad [14]$$

Fix a profile $\rho_0 : \mathbb{T}^d \to [0,1]$ bounded away from 0 and 1: $0 < \delta \leq \rho_0(u) \leq 1 - \delta$. Let $\rho(t,u)$ be the solution of the hydrodynamic equation [14] with initial condition ρ_0 and denote by $\nu_{\rho(t,\cdot)}^N$ the product

measure with slowly varying parameter associated to the profile $\rho(t, \cdot)$:

$$\nu^N_{\rho(t,\cdot)}\{\eta; \eta(x) = 1\} = \rho(t, x/N), \quad \text{for } x \in \mathbb{T}^d_N$$

Theorem 6 *Let $\{\mu^N : N \geq 1\}$ be a sequence of probability measures on $\mathcal{E}_N$ whose entropy with respect to $\nu^N_{\rho_0(\cdot)}$ is of order $o(N^d)$:*

$$H_N\left(\mu^N | \nu^N_{\rho_0(\cdot)}\right) = o(N^d)$$

Then, the relative entropy of the state of the process at the macroscopic time t with respect to $\nu^N_{\rho(t,\cdot)}$ is also of order $o(N^d)$:

$$H_N\left(\mu^N S^N_t | \nu^N_{\rho(t,\cdot)}\right) = o(N^d) \quad \textit{for every } t \geq 0$$

It is not difficult to deduce from this result a strong version of the hydrodynamic limit behavior of the interacting particle system:

Corollary 1 *Under the assumptions of the theorem, for every cylinder function Ψ and every continuous function $H : \mathbb{T}^d \to \mathbb{R}$,*

$$\lim_{N\to\infty} E_{\mu^N S^N_t}\left[\left| N^{-d} \sum_{x\in\mathbb{T}^d_N} H(x/N)\tau_x\Psi(\eta) - \int_{\mathbb{T}^d} H(u)\tilde{\Psi}(\rho(t,u))\,\mathrm{d}u \right|\right] = 0$$

The relative entropy method can be extended to nongradient systems and to asymmetric processes, whose macroscopic evolution is described by quasilinear hyperbolic equations, up to the first shock.

The hydrodynamic behavior of an interacting particle system corresponds to a law of large numbers for the empirical measure. The central limit theorem is well understood in equilibrium, but remains to this date an important open question in nonequilibrium. The large deviations for diffusive systems have also been investigated, as well as the hydrodynamic behavior of systems in contact with reservoirs. The Navier–Stokes equations have been derived as a correction of the hydrodynamic equation of asymmetric particle systems. We refer to Kipnis and Landim (1999) for further details.

See also: Boltzmann Equation (Classical and Quantum); Bose–Einstein Condensates; Breaking Water Waves; Fourier Law; Interacting Stochastic Particle Systems; Macroscopic Fluctuations and Thermodynamic Functionals; Multi-Scale Approaches.

Further Reading

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Interacting Stochastic Particle Systems

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Introduction

According to the basic principles of mechanics, the motion of atoms and molecules is governed, in the semiclassical approximation, by the deterministic Hamiltonian equations of motion. While all evidence points in this direction, for many problems this Hamiltonian approach is so complicated that it hardly yields any useful results. A simple example are many (10^9) polystyrene balls (size $1\,\mu\text{m}$) immersed in water. The Hamiltonian description would have to deal with the degrees of freedom of all the fluid molecules and all the polystyrene balls. Clearly, a more useful approach is to collect the incessant bombardment of a polystyrene ball by water molecules into a stochastic force acting on the ball with postulated statistical properties. For example, following Einstein, one could regard successive collisions as independent and occurring after an exponentially distributed waiting time. In addition to such stochastic forces, the polystyrene balls are charged and interact with each other through the screened Coulomb force.

On the one-particle level, stochastic models have a long tradition within statistical physics. Considerable part of the classical theory of Markov processes is the mathematical response to such type of description. The aspect of interaction is more recent. Its origin can be traced back to the Metropolis algorithm in early computer simulations ($\cong$1953). It was recognized that the Hamiltonian dynamics is a rather slow tool to statistically sample the Gibbs equilibrium distribution $Z^{-1}\exp[-H/k_BT]$. A more efficient route is to devise a stochastic algorithm which has as its unique stationary measure the Gibbs distribution. Such schemes are now known as Markov Chain Monte Carlo and of extremely wide use, not only in statistical physics but also in quantum chromodynamics (QCD) and other quantum field theories. The time appearing in the stochastic algorithm has no physical significance; it merely counts how often a certain operation is performed.

The second clearly identifiable push toward the use of interacting stochastic particle systems came from the study of critical dynamics. Close to a point of second-order phase transition, the equilibrium properties are very effectively handled by means of statistical field theories. Thus, it was natural to search for an extension into the time domain, which then led to time-dependent Ginzburg–Landau theories, where now time refers to physical time. These are interacting stochastic models, where one keeps only a few basic fields, together with their behavior under time reversal, their vector character, and whether they are dynamically conserved or not.

In probability theory, interacting stochastic particle systems date back to the seminal papers by M Kac in 1956 and independently by R L Dobrushin and by F Spitzer in 1970. Spitzer was motivated by spin-flip and spin-exchange dynamics, while Dobrushin had the vision of many locally interacting components. In the early days, one of the prime goals was the construction of the stochastic process in infinite volume, an enterprise which had important mathematical spin-off, for example, the theory of Dirichlet forms on function spaces. Physical models offer a rich menu to the probabilist, but there is also considerable input from other areas. To give just one example: in queueing theory one considers queues in series, that is, a customer served at one counter immediately moves on to the next one. If one regards as field the number of customers at each counter, one has an interacting stochastic particle system, the interaction being mediated through the servers.

This article is split into two sections. In the first one, we list and explain a few prototypical interacting stochastic particle systems. Of course, the list is hardly exhaustive and we restrict ourselves from the outset to models from statistical physics. In the second part, we summarize prominent lines of recent research. Again the wealth of material is overwhelming and we draw the line according to the rules of mathematical physics.

Model Systems

Our list is determined by the intrinsic mathematical properties of the stochastic particle system. Alternatively, a classification is possible according to the physical system, which would, however, be less transparent for our purposes. We restrict ourselves to models with only position-like degrees of freedom, but if needed velocity-like fields may be included. The most basic distinction is the behavior under time reversal. A model is called (statistically) "time reversible" if a particular history and its time-reversed image have the same probability. Technically, one imposes this through the condition of detailed balance. Nonreversible systems are much less explored, but currently a very active area of research.

Reversible Models

1. *Spin-flip, Glauber dynamics.* One considers spins attached to the sites of a regular lattice, which for symplicity we take as the hypercubic lattice $\mathbb{Z}^d$. The spin at site $x \in \mathbb{Z}^d$ is denoted by $\sigma_x = \pm 1$ and the whole spin configuration is denoted by σ. Thus, the state space of the Markov processs is $\{-1,1\}^{\mathbb{Z}^d} = \Omega$. Spin configurations evolve in time through random spin flips, that is, through a change from σ_x to $-\sigma_x$ according to configuration-dependent rates $c_x(\sigma)$. $c_x(\sigma)$ is local, in the sense that it depends only on the spins close to x, and is translation invariant, that is, if τ_y is the shift by y, then $c_{x+y}(\tau_y\sigma) = c_x(\sigma)$. If the current spin configuration is $\sigma(t)$, then after a short time $\mathrm{d}t$

$$\sigma_x(t+\mathrm{d}t) = \begin{cases} \sigma_x(t) & \text{with probability } 1 - c_x(\sigma(t))\,\mathrm{d}t \\ -\sigma_x(t) & \text{with probability } c_x(\sigma(t))\,\mathrm{d}t \end{cases}$$

The update is performed independently at each lattice site. Technically, it is more concise to specify the generator, L, of the Markov process. It acts on local functions $f:\Omega \to \mathbb{R}$ and is given by

$$Lf(\sigma) = \sum_{x\in\mathbb{Z}^d} c_x(\sigma)(f(\sigma^x) - f(\sigma)) \qquad [1]$$

where σ^x denotes the configuration σ with the spin at site x reversed. The transition probability from the configuration σ to the configuration σ' in time $t \geq 0$ is given by the matrix element $(\mathrm{e}^{Lt})_{\sigma,\sigma'}$ of the Markov semigroup e^{Lt}.

To impose time reversibility, one needs an energy function $H(\sigma)$ constructed according to the rules of equilibrium statistical mechanics. The condition of detailed balance then reads

$$c_x(\sigma) = c_x(\sigma^x)\mathrm{e}^{-\beta(H(\sigma^x)-H(\sigma))} \qquad [2]$$

with $\beta = 1/k_\mathrm{B}T$ the inverse temperature. Note that on the right only energy differences appear, which are always well defined. In finite volume the unique invariant measure is the Gibbs measure $Z^{-1}\mathrm{e}^{-\beta H}$.

2. *Spin-exchange, Kawasaki dynamics, stochastic lattice gases.* We model particles hopping on the lattice $\mathbb{Z}^d$ and switch to the occupation variables η_x, where $\eta_x = 0$ stands for site x empty and $\eta_x = 1$ stands for site x occupied. The state space is $\Omega = \{0,1\}^{\mathbb{Z}^d}$. Since the number of particles is conserved, the basic dynamical process is a random jump of a particle from x to a nearby site y, provided $\eta_y = 0$. Therefore, we specify the exchange rates $c_{xy}(\eta)$ between x and y. They are local, translation invariant and symmetric, that is, $c_{xy}(\eta) = c_{yx}(\eta)$. The generator now reads

$$Lf(\eta) = \frac{1}{2}\sum_{x,y\in\mathbb{Z}^d} c_{xy}(\eta)(f(\eta^{xy}) - f(\eta)) \qquad [3]$$

where η^{xy} is the configuration η with the occupancies at sites x and y exchanged.

The condition of detailed balance refers to the exchange and reads

$$c_{xy}(\eta) = c_{xy}(\eta^{xy})\mathrm{e}^{-\beta(H(\eta^{xy})-H(\eta))} \qquad [4]$$

In [4] we can freely add to H the chemical potential $-\mu\sum_x \eta_x$. Thus for stochastic lattice gases there is a one-parameter family of invariant measures, labeled by the chemical potential μ.

3. *Interacting Brownian motions.* These motions model, for example, suspensions as mentioned in the "Introduction". One considers a box $\Lambda \subset \mathbb{R}^d$ containing N Brownian particles. The jth Brownian particle has position $x_j \in \Lambda$. Thus, the state space of the Markov process is Λ^N. We assume that the Brownian particles interact through a (sufficiently local) even pair potential U. Then the total potential energy is

$$H(\underline{x}) = \frac{1}{2}\sum_{i,j=1}^{N} U(x_i - x_j), \quad \underline{x} = (x_1, \ldots, x_N) \qquad [5]$$

The dynamics of the Brownian particles is given through the stochastic differential equations

$$\mathrm{d}x_j(t) = -\sum_{i=1,i\neq j}^{N} \nabla U(x_j(t) - x_i(t))\,\mathrm{d}t + \sqrt{2D_0}\mathrm{d}W_j(t), \quad j = 1,\ldots,N \qquad [6]$$

$W_j(t), j = 1,\ldots,N$, are a collection of independent Brownian motions and D_0 is the diffusion coefficient of a single Brownian particle. Equation [6] has to be supplemented with suitable boundary conditions at the surface $\partial\Lambda$. Since the forces in [6] are the gradient of a potential, time reversibility is automatically satisfied with the invariant measure being $Z_N^{-1}\exp(-H(\underline{x})/D_0)\,\mathrm{d}x_1\cdots\mathrm{d}x_N$.

4. *Ginzburg–Landau models.* Ginzburg–Landau models should be viewed as discretized versions of stochastic partial differential equations. At every lattice site $x \in \mathbb{Z}^d$, there is a real-valued field $\phi_x \in \mathbb{R}$, a field configuration being denoted by ϕ. Formally, the state space is $\mathbb{R}^{\mathbb{Z}^d}$. Since the single-site space is noncompact, some growth condition at

infinity must be imposed. Next we give ourselves an energy, $H(\phi)$, one standard example being

$$H(\phi) = \sum_{x,y \in \mathbb{Z}^d, |x-y|=1} (\phi_x - \phi_y)^2 + \sum_{x \in \mathbb{Z}^d} V(\phi_x) \quad [7]$$

The on-site potential increases sufficiently rapidly, so as to make large field values unlikely. The ϕ-field evolves according to the set of stochastic differential equations

$$\mathrm{d}\phi_x(t) = -\frac{\partial H}{\partial \phi_x}(\phi(t))\mathrm{d}t + \sqrt{2/\beta}\,\mathrm{d}W_x(t), \quad x \in \mathbb{Z}^d \quad [8]$$

where $\{W_x(t), x \in \mathbb{Z}^d\}$ is a collection of independent Brownian motions. If $V(\phi_x) = \phi_x^2$, then $\phi(t)$ is a Gaussian field theory. To have an Ising-type phase transition, one would have to choose $V(\phi_x) = \lambda\phi_x^2 + \phi_x^4$.

It is rather simple to modify [8] as to incorporate a conservation law. To each directed bond (x, y), $|x - y| = 1$, one associates the current $j_{xy} = -j_{yx}$. If e is a unit vector, $|e| = 1$, then

$$\mathrm{d}\phi_x(t) + \sum_{e,|e|=1} j_{xx+e}(t)\mathrm{d}t = 0, \quad x \in \mathbb{Z}^d \quad [9]$$

The current has both a deterministic part, given through the gradient of a chemical potential, and a random part:

$$j_{xy}(t)\mathrm{d}t = -\left(\frac{\partial H}{\partial \phi_x} - \frac{\partial H}{\partial \phi_y}\right)(\phi(t))\mathrm{d}t + \mathrm{d}W_{xy}(t), \quad |x - y| = 1 \quad [10]$$

where $W_{xy}(t) = -W_{yx}(t)$ is a collection of independent Brownian motions labeled by nearest-neighbor bonds. The conserved quantity is $\sum_x \phi_x$. Again, the dynamics has a one-parameter family of stationary measures labeled by the "magnetic field". Since in [8] and [10] the drift is the gradient of a potential, Ginzburg–Landau models are reversible.

5. *Interface dynamics*. The scalar field ϕ describes the location of an interface. The energy of an interface does not depend on its absolute displacements. Thus, interface models are special Ginzburg–Landau models, which have an energy $H(\phi)$ invariant under the global shift $\phi_x \to \phi_x + a$ for all $x \in \mathbb{Z}^d$. An example is

$$H(\phi) = \sum_{x,y \in \mathbb{Z}^d, |x-y|=1} V(\phi_x - \phi_y) \quad [11]$$

with even V. Note that in order to have a normalizable equilibrium measure, the interface must be pinned somewhere.

6. *Several components*. For lattice gases, there may be several components. In a Ginzburg–Landau theory instead of a scalar, Ising-like field, one could consider a vector-valued, Heisenberg-like, field and require the energy to be invariant under global rotations of the field variables. The construction is as before and we do not have to repeat it.

7. *Constrained, glassy dynamics*. The constraint is enforced by setting some of the rates equal to zero. For example, in the case of standard Glauber dynamics, one could allow for a spin-flip only if at least two neighboring spins have the opposite sign. The Gibbs measure is still invariant, but the approach to equilibrium will be slowed down due to the constraint. It may even happen that the configuration space splits into several invariant subsets.

After this long and still incomplete list, let us turn to the nonreversible models.

Nonreversible Models

Mathematically, one merely has to drop the condition of detailed balance. To have a more concrete example, let L_i be the generator for the Glauber dynamics satisfying detailed balance with inverse temperature $\beta_i, i = 1, 2$. Then $L = L_1 + L_2$ generates a nonreversible dynamics provided $\beta_1 \neq \beta_2$. Physically, it corresponds to coupling the spins to two bulk thermal reservoirs of different temperatures. Our example leads to a general point which should be noted: While reversible models have a wide range of physical applicability, for nonreversible models nonequilibrium conditions have to be maintained over sufficiently long time spans, which poses considerable difficulties experimentally. Thus on a theoretical level, the efforts go into exploring properties of, say, semirealistic models.

Very roughly there are two broad classes of nonreversible models.

Boundary-driven models We consider a finite volume Λ. Inside Λ the dynamics is reversible as explained before. At the boundary $\partial\Lambda$ the system is coupled to particle, resp. energy, reservoirs. In case the boundary chemical potential, resp. temperature, is not uniform, the dynamics is nonreversible. To be more concrete let us reconsider the lattice gas discussed in item (2) (see the discussion following eqn [2]). Inside Λ the generator L_Λ is given by [3] and satisfies detailed balance [4]. The boundary generator is

$$L_{\partial\Lambda} f(\eta) = \sum_{x \in \partial\Lambda} c_x(\eta)(f(\eta^x) - f(\eta)) \quad [12]$$

where the notation is as in [1] with $\{-1, 1\}$ substituted by $\{0, 1\}$. $c_x(\eta)$ satisfies [2] with the same β as in the bulk, but a chemical potential μ_x depending on $x \in \partial\Lambda$. μ_x controls the injection/

absorption of particles at x. The generator for the nonreversible dynamics is then

$$L = L_\Lambda + L_{\partial\Lambda} \qquad [13]$$

Bulk-driven models A prototype is the two-temperature model mentioned above. More widely studied is a nonconservative force acting globally. Here the standard example are particles moving in Λ with periodic boundary conditions and subject to an additional uniform force field of strength F, which clearly cannot be written as the gradient of a potential. In the case of Brownian particles, by changing to a comoving frame of reference, one would be back to the reversible case $F = 0$. For lattice gases the lattice provides a fixed frame and the driven model has properties very different from the undriven one. This leads us to:

8. *Driven lattice gases.* The generator L is still given by [3]. Formally, we insert in [4] instead of H the Hamiltonian $H(\eta) - \sum_x (F \cdot x)\eta_x$. The exchange rates then satisfy the condition of "local" detailed balance as

$$c_{xy}(\eta) = c_{xy}(\eta^{xy})\, e^{-\beta(H(\eta^{xy}) - H(\eta))} \times e^{-\beta(F\cdot(x-y))(\eta_x - \eta_y)} \qquad [14]$$

This means, particles preferentially jump in the direction of F. On the infinite lattice the dynamics admits two classes of stationary measures. First, there is the Gibbs measure with particles piling up along F and formally given by

$$Z^{-1} e^{-\beta(H(\eta) - \sum_x (F\cdot x)\eta_x)} \qquad [15]$$

With respect to this measure the dynamics is reversible. Second, there are translation invariant measures with nonzero steady-state current. This cannot happen for reversible models. A very widely studied particular case is the asymmetric simple exclusion process for which $d = 1, H(\eta) = 0$, and jumps are only to nearest-neighbor sites.

Items of Interest

As there are thousands of research papers in mathematical physics alone, it is literally impossible to provide any sort of summary. On the other hand, the type of questions investigated are generic. Thus, we just explain what one would like to understand without paying much attention to the fractal boundary between "proven" and "unproven." For the construction of the stochastic processes listed above, there is a well-developed probabilistic theory available. Thus, the main focus is on "qualitative properties" of the stochastic particle system. As in the previous section, we distinguish between reversible and nonreversible models.

Reversible Models

1. *Equilibrium state.* The most basic question concerns the classification of invariant measures in infinite volume. By construction, they are the Gibbs measures for the Hamiltonian appearing in the condition of detailed balance. In principle there could be more, which so far has been excluded only in dimension 1 or 2. Properties of the invariant measure belong to the domain of equilibrium statistical mechanics.

Thus we can turn directly to:

2. *Spectral analysis of the generator L.* We fix some extreme Gibbs measure stationary for L. By detailed balance, e^{Lt} is a symmetric Markov semigroup in $L^2(\Omega, \mu)$. Hence, L is self-adjoint and $L \leq 0$. Furthermore, it has a nondegenerate eigenvalue 0. The rate of approach to equilibrium is determined by the spectral gap of L. Related are log-Sobolev inequalities which serve as a stronger notion. For models with a conservation law, there is no spectral gap. Thus, the more appropriate question is to study how fast the gap vanishes as the volume Λ increases. In the case of independent components, the spectral subspaces for L are organized as single excitation, double excitation etc. Such a structure persists as the interaction is turned on which, on a mathematical level, is similar to the particle spectrum of a quantum field theory.

Physically more directly relevant are:

3. *Spacetime correlations.* To be concrete, let us consider a Ginzburg–Landau field theory $\phi_x(t)$ starting with a translation invariant Gibbs measure μ. Then $\phi_x(t)$ is a spacetime stationary process. The two-point correlation function is the covariance

$$\langle \phi_x(t)\phi_0(0)\rangle - \langle \phi_0(0)\rangle^2 \qquad [16]$$

Its Fourier transform is directly linked to energy–momentum resolved scattering intensity from a probe which is modeled by the respective Ginzburg–Landau theory. For $t = 0$, the expression [16] is the static correlation, again belonging to the domain of equilibrium statistical mechanics. The time decay depends on whether the field is dynamically conserved or not.

Correlation functions do not always capture the physics of the system well. This is certainly true for:

4. *Dynamics at low temperatures.* Let us consider the Glauber dynamics for the ferromagnetic Ising model in the finite but large volume Λ. Then there is a very high free energy barrier between configurations typical for the + phase and those typical for the − phase. If one starts the spin system in the + phase, one

may study through which configurations the system moves to the − phase and how much time such a process will take. If the two phases are symmetric with the external magnetic field $h = 0$, the spin system tunnels, while for $h < 0$ and small the + phase is metastable. Another widely studied situation, also experimentally, is the quenching from high to low temperatures. In our context this means that the initial measure is Bernoulli, while the Glauber dynamics runs at low temperatures. Then spin clusters coarsen as time proceeds developing well-defined interfaces which are governed through motion by mean curvature.

Close to a point of second-order phase transition, one has to deal with:

5. *Critical dynamics*. The usual Glauber dynamics becomes very slow at the critical point and reliable equilibrium is hard to achieve. It is thus a challenge to design faster algorithms. One proposal is the Swendsen–Wang algorithm which is based on the Fortuin–Kasteleyn representation and flips a whole cluster of spins simultaneously.

So far we concentrated on statistical properties. Researchers have been fascinated by the observation that for stochastic particle systems, the transition to a deterministic macroscopic evolution can be handled with full rigor. Such a program has been baptized:

6. *Hydrodynamic limit*, which is meaningful only for particle systems with one or several conservation laws. Let us discuss then a reversible lattice gas with Hamiltonian H. We start the dynamics with a state of local equlibrium which is Gibbs with a slowly varying chemical potential, that is,

$$Z^{-1}\exp\left[-\beta\left(H(\eta)-\sum_{x}\mu(\varepsilon x)\eta_x\right)\right], \quad \varepsilon \ll 1 \quad [17]$$

Such a measure is almost time invariant. For small ε, at least approximately, such a structure should persist in the course of time at the expense of properly regulating the chemical potential. For our example, the correct timescale is $\varepsilon^{-2}t$ in microscopic units, and the evolution equation for the density, related thermodynamically to the chemical potential, is a nonlinear diffusion equation of the form

$$\frac{\partial}{\partial t}\rho_t = \nabla \cdot D(\rho_t)\nabla\rho_t \quad [18]$$

We turn to the nonreversible models.

Nonreversible Models

While for reversible models the study of the stationary Gibbs measure is its own field of inquiry, here the first entry must be:

7. *Nonequilibrium steady state*. This steady state is determined through the dynamics, since the stationary measure μ has to satisfy $\mu(Lf) = 0$ for a sufficiently large class of functions f. As in equilibrium, phase transitions may occur. In the nonconservative case it would mean that the infinitely extended system has several extreme stationary measures. In the conservative case, say with the density as locally conserved field, it would mean that there is an interval of densities for which there is no extreme stationary measure. Given the nonequilibrium steady state, one may wonder about its typical fluctuations and large deviations. In contrast to thermal equilibrium, weak long-range correlations are the rule.

8. *Spacetime correlations in the steady state*. Through the bulk drive the power-law decay of time correlations may change. For example for the symmetric and asymmetric exclusion process, the steady states are Bernoulli with density ρ, denoted by $\langle\cdot\rangle_\rho$. For the on-site density–density correlation, one finds, for large t,

$$\langle\eta_0(t)\eta_0(0)\rangle_{1/2} - \frac{1}{4} \cong \begin{cases} t^{-1/2} & \text{for } F = 0 \\ t^{-2/3} & \text{for } F \neq 0 \end{cases} \quad [19]$$

9. *Hydrodynamic limit*. The concept of slowly varying conserved fields remains valid; only local equilibrium must be replaced by local stationarity. Generically, there are nonzero currents in the steady state. Therefore, the macroscopic fields change on the timescale $\varepsilon^{-1}t$ (cf. item (5)) and are governed by a hyperbolic conservation law of the form

$$\frac{\partial}{\partial t}\rho_t + \operatorname{div} j(\rho_t) = 0 \quad [20]$$

in the case of a single conservation law. Here, $j(\rho)$ is the average steady state in the stationary measure at density ρ. Several conservation laws have an intriguing rich variety of solutions. Even on the level of continuum partial differential equations, such systems of hyperbolic conservation laws still pose unresolved basic problems.

See also: Ginzburg–Landau Equation; Glassy Disordered Systems: Dynamical Evolution; Interacting Particle Systems and Hydrodynamic Equations; Macroscopic Fluctuations and Thermodynamic Functionals; Stochastic Differential Equations.

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Interfaces and Multicomponent Fluids

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Introduction

Many important industrial problems involve flows with multiple constitutive components. Examples include extractors, separators, reactors, sprays, polymer blends, and microfluidic applications such as DNA analysis, and protein crystallization. Due to inherent nonlinearities, topological changes, and the complexity of dealing with unknown, active, and moving surfaces, multiphase flows are challenging. Much effort has been put into studying such flows through analysis, asymptotics, and numerical simulation. Here, we focus on review on studies of multicomponent fluids using continuum numerical methods.

There are many ways to characterize moving interfaces. The two main approaches to simulating multiphase and multicomponent flows are interface tracking and interface capturing. In interface-tracking methods (examples include boundary-integral, volume-of-fluid, front-tracking, immersed-boundary, and immersed-interface methods), Lagrangian (or semi-Lagrangian) particles are used to track the interfaces. In (BIMs), the flow equations are mapped from the immiscible fluid domains to the sharp interfaces separating them thus reducing the dimensionality of the problem (the computational mesh discretizes only the interface). In interface-capturing methods such as level-set and phase-field methods, the interface is implicitly captured by a contour of a particular scalar function.

The equations governing the motion of an unsteady, viscous, incompressible, immiscible two-fluid system are the Navier–Stokes equations (the subscript i denotes the ith flow component):

$$\rho_i\left(\frac{\partial \boldsymbol{u}_i}{\partial t} + \boldsymbol{u}_i \cdot \nabla \boldsymbol{u}_i\right) = \nabla \cdot \sigma_i + \rho_i \boldsymbol{g}, \quad i = 1,2 \qquad [1]$$

$$\sigma_i = -p_i \boldsymbol{I} + 2\eta_i \boldsymbol{D}_i \qquad [2]$$

where ρ_i is the density, $\boldsymbol{u}_i$ is the fluid velocity, p_i is the pressure, η_i is the viscosity, and $\boldsymbol{g}$ is the gravitational acceleration vector. In eqn [2], σ_i is the stress tensor, $\boldsymbol{I}$ is the identity matrix, and $\boldsymbol{D}_i$ is the rate of deformation tensor and defined as $\boldsymbol{D}_i = (1/2)(\nabla \boldsymbol{u}_i + \nabla \boldsymbol{u}_i^{\mathrm{T}})$. The velocity field is subject to the incompressibility constraint,

$$\nabla \cdot \boldsymbol{u}_i = 0 \qquad [3]$$

We let Γ denote the fluid interface. The effect of surface tension is to balance the jump of the normal stress along the fluid interface. This gives rise to a Laplace–Young condition for the discontinuity of the normal stress across Γ:

$$[\sigma \boldsymbol{n}]_\Gamma = \tau \kappa \boldsymbol{n} \qquad [4]$$

where $[\sigma]_\Gamma$ denotes the jump $\sigma_2 - \sigma_1$ across Γ, κ is the curvature of Γ (positive for a spherical interface), τ is the surface tension coefficient which is assumed to be constant, and $\boldsymbol{n}$ is the unit normal vector along Γ directed toward fluid 2. The fluid velocity is continuous across Γ.

In order to circumvent the problems associated with implementing the Laplace–Young calculation at the exact interface boundary, Brackbill and collaborators developed a method referred to as the continuum surface force (CSF) method. See the review by Scardovelli and Zaleski (1999). In this method, the surface tension jump condition is converted into an equivalent singular volume force that is added to the Navier–Stokes equations. Typically, the singular force is smoothed and acts only in a finite transition region across the interface. The system of equations [1]–[2] and the boundary condition, eqn [4] can be combined into the following distribution formulation that holds in both phases:

$$\rho(\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) = -\nabla p + \nabla \cdot (2\eta \boldsymbol{D}) + \rho \boldsymbol{g} + \boldsymbol{F}_{\text{sing}}, \quad \nabla \cdot \boldsymbol{u} = 0 \qquad [5]$$

where the subscript i is dropped (i.e., it is understood that $\boldsymbol{u} = \boldsymbol{u}_i$ in fluid i, etc.,) and $\boldsymbol{F}_{\text{sing}}$ is singular

surface tension force that is given by $F_{\text{sing}} = -\tau\kappa\delta_\Gamma n$, where δ_Γ is the surface delta-function.

Numerical Methods for Multicomponent Fluid Flows

Interface-Tracking Methods

Boundary-integral methods (BIMs) BIMs can be highly accurate for modeling free surface flows with relatively regular interface topologies. The BIM was apparently first used by Rosenhead in 1932 to study vortex sheet roll-up. In this approach, the interface is explicitly tracked, but the flow solution in the entire domain is deduced solely from information possessed by discrete points along the interface.

BIMs have been used for both inviscid and Stokes flows. For a review of Stokes flow computations, see Pozrikidis (2001), and for a review of computations of inviscid flows, see Hou *et al.* (2001). For flows with both inertia and viscosity, volume integrals must be incorporated into the formulation.

When inertial forces are negligible (left-hand side term of eqn [1] is dropped), the velocity $u(x_0)$ at a given point x_0 on the interface can be obtained by means of the boundary-integral formulation,

$$(\lambda+1)u(x_0) = 2u_\infty(x_0) - \frac{1}{4\pi}\int_\Gamma f(x)G(x_0,x) \times n(x)\,\mathrm{d}s(x) \qquad [6]$$

$$-\frac{\lambda-1}{4\pi}\int_\Gamma u(x)\cdot T(x_0,x)\cdot n(x)\,\mathrm{d}s(x) \qquad [7]$$

where λ is the viscosity ratio, u_∞ is an imposed velocity prevailing in the absence of the interfaces, and $f(x)$ is the capillary force function $f = \tau\kappa$. The tensors G and T are the Stokeslet and stresslet, respectively:

$$G(x_0,x) = \frac{I}{r} + \frac{\hat{x}\hat{x}}{r^3}$$
$$T(x_0,x) = -\frac{6\hat{x}\hat{x}\hat{x}}{r^5} \qquad [8]$$

$$\text{where } \hat{x} = x - x_0, \quad r = |\hat{x}| \qquad [9]$$

The boundary conditions at the interface, that is, the stress balance equation [4] and continuity of the velocity across the interface, are automatically satisfied by the boundary-integral formulation.

The normal velocity of the interface $\Gamma(x,t)$ is given by

$$\frac{\mathrm{d}x}{\mathrm{d}t}\cdot n(x) = u(x,t)\cdot n(x) \qquad [10]$$

The shape of the interface does not depend on the tangential velocity and there are many possible choices that can be taken, see Hou *et al.* (2001).

The principal advantages gained by using BIMs are the reduction of the flow problem by one dimension since the formulation involves quantities defined on the interface only and the potential for highly accurate solutions if the flow has topologically regular interfaces. In addition, highly efficient adaptive surface mesh refinement algorithms have recently been developed to improve the performance and accuracy of the methods (Cristini *et al.* 2001). The main disadvantages are the development of accurate quadratures of integrals with singular kernels (particularly in 3D) and the need for local surgery of the interface in the event of topological changes.

BIMs have been successfully used for simulations of complex multiphase flows: drop deformation and breakup; jets; capillary waves; mixing; drop-to-drop interaction; suspension of liquid drops in viscous flow (e.g., see Cristini *et al.* (2001), Hou *et al.* (2001), and Pozrikidis (2001) and the references therein).

Volume-of-fluid (VOF) method In the VOF method (see Scardovelli and Zaleski (1999) for a recent review), the location of the interface is determined by the volume fraction c_{ij} of fluid 1 in the computational cell, Ω_{ij}. In cells containing the interface $0 < c_{ij} < 1$, $c_{ij} = 1$ in cells containing fluid 1, and $c_{ij} = 0$ in cells containing fluid 2 as shown in **Figure 1b**.

A VOF algorithm is divided into two parts: a reconstruction step and a propagation step. A typical interface reconstruction is shown in **Figure 1c**. In the piecewise linear interface construction (PLIC) method, the true interface, as shown in **Figure 1a**, is approximated by a straight line perpendicular to an interface normal vector n_{ij} in each cell Ω_{ij}. The normal vector n_{ij} is determined from the volume fraction gradient using data from neighboring cells. With given a volume fraction c_{ij}

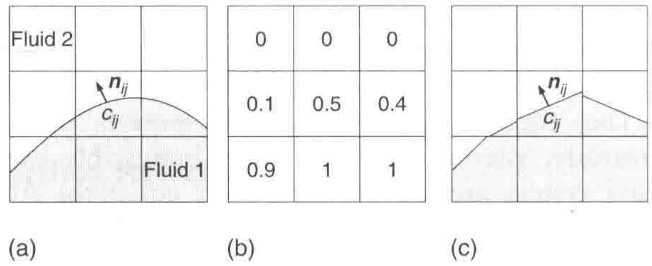


Figure 1 VOF representation of an interface: (a) actual interface, (b) volume fraction, and (c) an approximation to the interface is produced using an interface reconstruction method such as piecewise linear approximation as shown.

and a normal vector $\boldsymbol{n}_{ij}$, the interface is given by the straight line with normal $\boldsymbol{n}_{ij}$ such that area beneath the line in cell Ω_{ij} is equal to c_{ij}. More recently, parabolic reconstructions of the interface have been used to gain higher-order accuracy for the surface tension force (e.g., the "parabolic reconstruction of surface tension" or PROST algorithm).

Once the interface has been reconstructed, its motion by the underlying flow field must be modeled by a suitable advection algorithm. The key here is that the explicit interface reconstruction enables fluxes to be developed that exactly conserve mass and do not diffuse the interface.

Capillary effects may be represented by the continuous surface stress (Scardovelli and Zaleski 1999),

$$\boldsymbol{T} = -\tau(\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n})|\nabla\tilde{c}|, \quad \boldsymbol{F}_{\text{sing}} = -\nabla \cdot \boldsymbol{T} \qquad [11]$$

where $\tilde{c}$ is a smoothed version of the volume fraction. For the flows in which the capillary force is the dominant physical mechanism, the PROST algorithm discussed above can be used to significantly reduce spurious currents due to inaccurate representation of surface tension terms and associated pressure jump in normal stress.

The distribution form of the fluid equations [5] is typically solved using a variant of the projection method for incompressible single phase flows.

VOF methods are popular and have been used in commercial multiphase flow codes, in models of inkjet printers, flows with surfactants and in many other applications (e.g., see Scardovelli and Zaleski (1999) and James and Lowengrub (2004) and the references therein). The principal advantage of VOF methods is their inherent volume-conserving property. Nevertheless, spurious bubbles and drops may be created. The reconstruction of the interface from the volume fractions and the computation of geometric quantities such as curvature are typically less accurate than other methods discussed here since the curvature and normal vectors are obtained by differentiating a nearly discontinuous function (volume fraction).

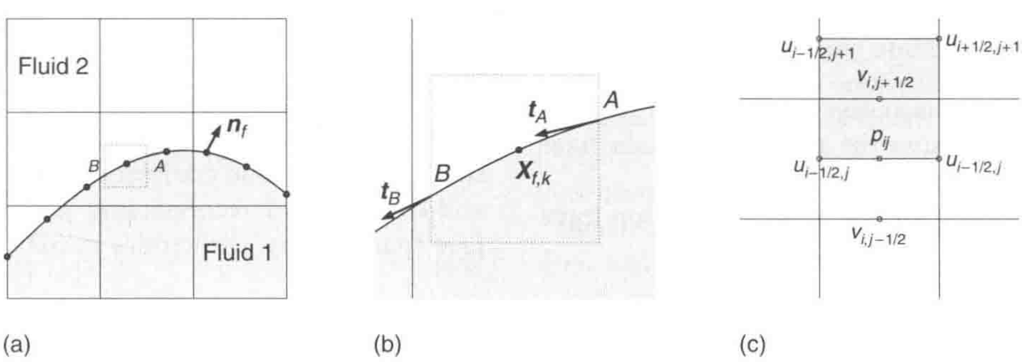
Front-tracking methods The basic idea behind the original front-tracking method is the use of two grids as illustrated in **Figure 2**. One is a standard, Eulerian finite difference mesh that is used to solve the fluid equations. The other is a discretized interface mesh that is used to explicitly track the interface and compute surface tension force which is then transferred to the finite difference mesh via a discrete delta-function. Front tracking was first proposed by Richtmyer and Morton and further developed by Glimm and co-workers.

A similar approach was taken by Unverdi and Tryggvason (see Tryggvason *et al.* (2001) and Peskin (2002) for recent reviews), who combined a moving grid description of the interface with flow computations on a fixed grid. In this immersed-boundary approach, all the fluid phases are treated together by solving a single set of governing equations. This method has its roots in the original marker-and-cell (MAC) method, where marker particles are used to identify each fluid and the immersed-boundary method of Peskin and McQueen, that was designed to track moving elastic boundaries in homogeneous fluids.

The interface is represented discretely by Lagrangian markers that are connected to form a front which lies within and moves through a stationary Eulerian mesh.

In Tryggvason's original implementation, the basic structural unit is a line segment. Since the interface moves and deforms during the computation, interface elements must occasionally be added or deleted to maintain regularity and stability. In the event of merging/breakup, elements must be relinked to effect a change in topology.

The interface is represented using an ordered list of marker particles $\boldsymbol{x}_k = ((x_1)_k, (x_2)_k), 1 \leq k \leq N$.



(a) (b) (c)

Figure 2 (a) The basic idea in the front-tracking method is to use two grids – a stationary finite difference mesh and a moving Lagrangian mesh, which is used to track the interface. (b). Blow-up of the subgrid control volume in (a). (c) Control volume for the Eulerian mesh, $\Omega_{i,j+(1/2)}$.

The first step in this algorithm is the advection of the marker particles. A simple bilinear interpolation is used to find the velocity inside each grid cell (indicated in **Figure 2c**). The marker particles are then advected in a Lagrangian manner. Once the points have been advected, a list of connected polynomials $(p_i^x(s), p_i^y(s))$ is constructed using the marker particles. This gives a parametric representation of the interface, with s typically an approximation of the arclength. Both lists are ordered and thus identify the topology of the interface. In later works, higher-order polynomials have been used (e.g., cubic splines) and semi-Lagrangian evolutions have been implemented where other tangential velocities have been used.

As the interface evolves, the markers drift along the interface following tangential velocities and more markers may be needed if the interface is stretched by the flow. Typically, the markers are redistributed along the interface to maintain an accurate interface representation.

Next, we compute the surface tension force,

$$F_{\text{sing}}(x,t) = \int_{\Gamma(t)} \tau\kappa_f \delta(x - x_f(s)) n_f \mathrm{d}s \qquad [12]$$

where the subscript f means values evaluated at the interface $\Gamma(t)$ and s is arclength. The discrete numerical implementation of this distribution onto the fixed grid is in the form of a sum over interface elements, $x_{f,k}$:

$$F_{ij}(x) = \sum_k f_k \delta(x - x_{f,k}) \Delta s_k \qquad [13]$$

where Δs_k is the average of the straight line distances from the point $x_{f,k}$ to the two neighboring points $x_{f,k+1}$ and $x_{f,k-1}$ as indicated by the subgrid control volume shown in **Figures 2a** and **2b**. The delta-function is typically taken to be Peskin's discrete Dirac delta-function:

$$\delta(x - x_{f,k}) = \begin{cases} \prod_{i=1}^{2} \frac{1}{4h}\left(1 + \cos\frac{\pi[x_i - (x_{f,i})_k]}{2h}\right) & \text{if } |x - x_{f,k}| \le 2h \\ 0 & \text{otherwise} \end{cases} \qquad [14]$$

Other higher-order alternative forms of the regularized delta-function using the product formula have recently been proposed.

Using the Frenet relation, the surface tension force on a short segment of the front is given by

$$f_k = \int_A^B \tau\kappa_f n_f \mathrm{d}s = \int_A^B \tau \frac{\partial t_f}{\partial s} \mathrm{d}s = \tau(t_B - t_A) \qquad [15]$$

where A and B are the segment endpoints that lie on the boundary of the subgrid control volume (**Figures 2a** and **2b**), and t_f is a tangent vector computed by fitting a polynomial to the endpoints of each element.

In the case of flows with varying density and/or viscosity between the fluid components, there is a need to calculate the phase indicator function $I(x,t)$ (defined by interface geometry and position), which has the value 0 in fluid 1 and 1 in fluid 2. The indication function can be determined via the solution of the equation

$$\Delta I(x,t) = \nabla \cdot \int_{\Gamma(t)} n_f \delta(x - x_f(s,t)) \mathrm{d}s \qquad [16]$$

This equation is discretized on the Eulerian mesh and a discrete delta-function (e.g., eqn [14]) is used. The fluid properties such as density and viscosity are determined via the indicator function, that is, $\rho(x,t) = \rho_1 + (\rho_2 - \rho_1) I(x,t)$, etc.

As in the volume of fluid algorithm, the distribution form of the Navier–Stokes equations [5] are typically solved using a version of Chorin's projection method.

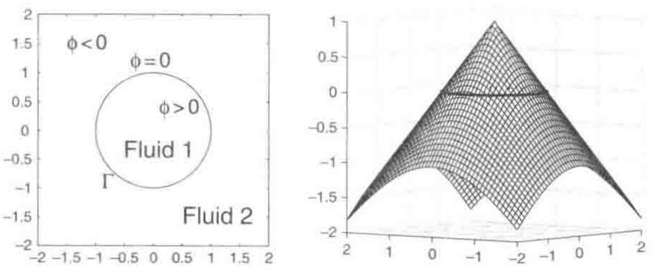
An alternative flow solver that can be used to integrate the flow equations in the presence of an interface is the immersed-interface method (IIM). The IIM was developed by Leveque and Li (see the review Li 2003), and can be used together with front-tracking as well as level-set methods.

The IIM directly incorporates jump conditions for the normal stress into the finite difference stencil. The key idea of this method is to use the jump conditions in Taylor series expansions of pressure and velocity near interfaces to derive difference equations that achieve pointwise second-order accuracy.

The principal advantage of front-tracking algorithms is their inherent accuracy, due in part to the ability to use a large number of grid points on the interface. Front-tracking methods can be complicated to implement, particularly in 3D, but give the precise location and geometry of the interface. In addition, explicit front tracking permits more than one interface to be present in a single computational cell without coalescence, which can be important in dense bubbly flows, emulsions, etc. One of major handicaps of front-tracking methods is the difficulty in modeling topological changes of the interface such as breakup and coalescence without *ad hoc* cut-and-connect and reconnecting parameterized interface (particularly, difficulties in 3D).

Interface-Capturing Methods

Level-set method Level-set methods, introduced by Osher and Sethian (see the recent review papers (Osher and Fedkiw 2001, Sethian and Smereka



(a) (b)

Figure 3 (a) Zero contour of ϕ representing the interface Γ. (b) Surface of ϕ with zero contour.

2003) and the recent texts (Osher and Fedkiw 2002, Sethian 1999)), are popular computational techniques for tracking moving interfaces. These methods rely on an implicit representation of the interface as the zero set of an auxiliary function (level-set function). The application of these methods to incompressible, multiphase flows started with the work of Osher, Merriman, Sussman, Smereka, Hou, and their collaborators.

In the level-set method, the level-set function $\phi(\boldsymbol{x}, t)$ is defined as follows (see **Figure 3**):

$$\phi(\boldsymbol{x}, t)\begin{cases} > 0 & \text{if } \boldsymbol{x} \in \text{fluid 1} \\ = 0 & \text{if } \boldsymbol{x} \in \Gamma \text{ (the interface between fluids)} \\ < 0 & \text{if } \boldsymbol{x} \in \text{fluid 2} \end{cases}$$

and the evolution of ϕ is given by

$$\phi_t + \boldsymbol{u} \cdot \nabla\phi = 0 \qquad [17]$$

which means that the interface moves with fluid.

To keep the interface geometry well resolved, the level-set function ϕ should be a distance function near the interface. However, under the evolution [17] it will not necessarily remain as such. We note that special velocity extensions $\boldsymbol{v}$ off the interface (i.e., $\boldsymbol{v} = \boldsymbol{u}$ at the interface, $\boldsymbol{v} \neq \boldsymbol{u}$ away from interface) have been recently developed to better maintain ϕ as a distance function (e.g., Sethian and Smereka (2003) and Macklin and Lowengrub (2005)). Typically, a reinitialization step (solving a Hamilton–Jacobi type equation, eqn [18]) below, is performed to keep ϕ as a distance function near the interface while keeping original zero-level set unchanged. More specifically, given a level-set function, ϕ, at time t, the contours are redistributed according to the steady-state solution of the equation

$$\frac{\partial d}{\partial \tau} = S_\epsilon(\phi)(1 - |\nabla d|), \quad d(\boldsymbol{x}, 0) = \phi(\boldsymbol{x}) \qquad [18]$$

where S_ϵ is the smoothed sign function defined as

$$S_\epsilon(\phi) = \frac{\phi}{\sqrt{\phi^2 + \epsilon^2}} \qquad [19]$$

where ϵ is usually is one or two grid lengths. After solving eqn [18] to steady state $\phi(\boldsymbol{x}, t)$ is then replaced by $d(\boldsymbol{x}, \tau_{\text{steady}})$. Note that $d(\boldsymbol{x}, \tau_{\text{steady}})$ is typically a good approximation of the signed distance function.

The density and viscosity are defined as

$$\rho(\phi) = \rho_2 + (\rho_1 - \rho_2)H_\epsilon(\phi)$$

and

$$\eta(\phi) = \eta_2 + (\eta_1 - \eta_2)H_\epsilon(\phi) \qquad [20]$$

where $H_\epsilon(\phi)$ is the smoothed Heaviside function given by

$$H_\epsilon(\phi) = \begin{cases} 0 & \text{if } \phi < -\epsilon \\ \frac{1}{2}\left[1 + \frac{\phi}{\epsilon} + \frac{1}{\pi}\sin(\pi\phi/\epsilon)\right] & \text{if } |\phi| \leq \epsilon \\ 1 & \text{if } \phi > \epsilon \end{cases}$$

The mollified delta-function is $\delta_\epsilon(\phi) = \mathrm{d}H_\epsilon/\mathrm{d}\phi$. The surface tension force is given as

$$\boldsymbol{F}_{\text{sing}} = -\tau\nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right)\delta_\epsilon(\phi)\frac{\nabla\phi}{|\nabla\phi|} \qquad [21]$$

The fluid equations [5] are solved using projection methods, the IIM or the ghost-fluid (GF) method (e.g., Osher and Fedkiw (2001, 2002) and Fedkiw *et al.* (2003)). The GF method is similar to the IIM in that jump discontinuities are incorporated in the finite difference stencil. In the GF algorithm, subcell resolution is used to mark the interface position and the values of discontinuous quantities are artificially extended to grid points neighboring the interface via extrapolation. A fully second order accurate GF method for moving interfaces has recently been developed (Macklin and Lowengrub 2005).

Applications of the level-set method include multiphase flows, viscoelastic fluid flows and fluid–structure interactions (e.g., see the reviews Osher and Fedkiw (2001, 2002), Sethian (1999), and Sethian and Smereka (2003)).

Advantages of the level-set algorithm include the simplicity with which it can be implemented, the ability to capture merging and breakup of interfaces automatically, and the ease with which the interface geometry can be described using the level-set function. A disadvantage of the level-set method is that mass is not conserved.

Accurate numerical simulations of multiphase flow and topology transitions require the computational mesh to resolve both the macroscales (e.g., droplet size, flow geometry) and the microscales to accurately capture local interface geometries near contact region, van der Waals forces, surfactant distribution, and Marangoni stresses. Adaptive mesh

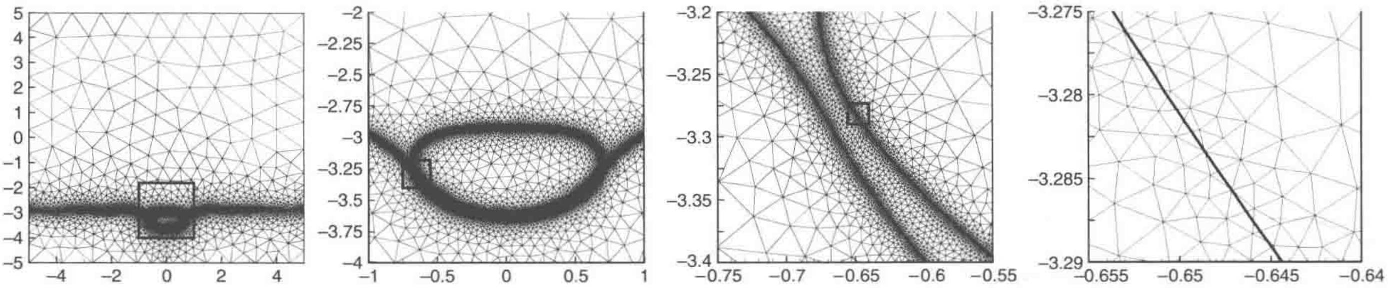


Figure 4 Each of the first three figures has a boxed region that is magnified in the next figure. The rates of magnification are 5, 10, 40/3, respectively. The meshes in the figure are used to simulate the drop-impacting interface problem. Source: Zheng X, Anderson A, Lowengrub JS, and Cristini V (unpublished).

algorithms have recently been used greatly to increase accuracy and computational efficiency in level-set methods. Typically, the methods involve Cartesian adaptive mesh refinement. Problems tackled using this approach include droplet formation in inkjet printers and wake development behind a ship. Another approach, recently developed, is to use adaptive unstructured mesh refinement (Zheng *et al.* 2005), as shown in **Figure 4**, in which the impact of a drop onto a fluid interface is captured.

Hybrid Methods

More recently, a number of hybrid methods, which combine good features of each algorithm, have been developed. These include coupled level-set volume-of-fluid (CLSVOF) algorithms, particle level-set methods, marker-VOF methods and level-contour front-tracking methods.

Level-set and VOF methods have recently been combined. The volume fraction is used to maintain volume conservation, while the level-set function is used to describe the interface geometry. After every time step, the volume-fraction function and level-set function are made compatible. The coupling between the level-set function ϕ and the VOF function c occurs through the normal of the reconstructed interface and through the fact that the level-set function is reset to the exact signed normal distance to the reconstructed interface (where the area below the reconstructed interface is given by the volume-fraction function).

In the particle level-set method, Lagrangian disconnected marker particles are randomly positioned near the interface and are passively advected by the flow in order to rebuild the level-set function in under-resolved zones, such as high-curvature regions and near filaments. In these regions, the standard nonadaptive level-set method regularizes excessively the interface structure and mass is lost. The use of marker particles significantly ameliorates these difficulties.

Recently, a hybrid method has been developed, which uses both marker particles, to reconstruct and move the interface, and the volume-fraction function to conserve volume. In this approach, a smooth motion of the interface, typical of marker methods is obtained together with volume conservation, as in standard VOF methods. This work improves both the accuracy of interface tracking, when compared to standard VOF methods, and the conservation of mass, with respect to the original marker method.

Finally, a hybrid method that combines a level contour reconstruction technique with front-tracking methods has recently been developed to automatically model the merging and breakup of interfaces in three-dimensional flows.

Phase-Field Method

Phase-field, or diffuse-interface, models are an increasingly popular choice for modeling the motion of multiphase fluids (see Anderson *et al.* (1998) for a recent review). In the phase-field model, sharp fluid interfaces are replaced by thin but nonzero thickness transition regions where the interfacial forces are smoothly distributed. The basic idea is to introduce a conserved order parameter (e.g., mass concentration) that varies continuously over thin interfacial layers and is mostly uniform in the bulk phases (see **Figure 5**).

For density-matched binary liquids (let $\rho = 1$ for simplicity), the coupling of the convective Cahn–Hilliard equation for the mass concentration with a modified momentum equation that includes a phase-field-dependent surface force is known as Model H (Hohenberg and Halperin 1977). In the case of fluids with different densities a phase-field model has been proposed by Lowengrub and Truskinovsky. Complex flow morphologies and topological transitions such as coalescence and interface breakup can be captured naturally and in a mass-conservative and energy-dissipative fashion since there is an associated free energy functional.

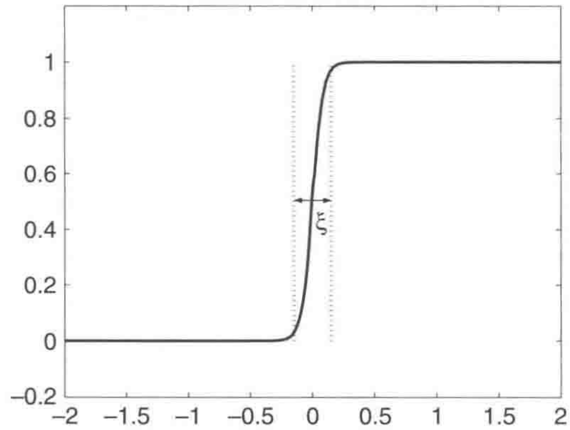


Figure 5 A concentration prome across an interface with interface thickness, ξ.

The phase field is governed by the following advective Cahn–Hilliard equation:

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = \nabla \cdot (M(c) \nabla \mu) \qquad [22]$$

$$\mu = F'(c) - \epsilon^2 \Delta c \qquad [23]$$

where $M(c) = c(1-c)$ is the mobility, $F(c) = (1/4)c^2(1-c)^2$ is a Helmholtz free energy that describe the coexistence of immiscible phases, and ϵ is a measure of interface thickness and $\epsilon \sim \xi$ (see **Figure 5**). It can be shown that in the sharp interface limit $\epsilon \to 0$, the classical Navier–Stokes system equations and jump conditions are recovered.

The singular surface tension force is $\boldsymbol{F}_{\text{sing}} = -6\sqrt{2}\tau\epsilon\nabla \cdot (\nabla c \otimes \nabla c)$, where τ is the surface tension coefficient. An alternative surface tension force formulation based on the CSF is $\boldsymbol{F}_{\text{sing}} = -6\sqrt{2}\tau\epsilon\nabla \cdot (\nabla c/|\nabla c|)|\nabla c|\nabla c$.

Recently, very efficient nonlinear multigrid methods have been developed to solve implicit discretizations of the Cahn–Hilliard equation (e.g., Kim *et al.* (2004)). These schemes have been combined with projection methods to solve the Navier–Stokes equations to perform simulations of multiphase flows.

An example of simulation of liquid thread breakup using a phase-field method is shown in **Figure 6**. A long cylindrical thread of a viscous fluid 1 is in an infinite mass of another viscous fluid 2. If the thread becomes varicose with wavelength λ, the equilibrium of the column is unstable, provided λ exceeds the circumference of the cylinder. This is the Rayleigh capillary instability that results in surface-tension-driven breakup of the thread.

An advantage of the phase-field approach is that it is straightforward to include more complex physical effects. For example, the binary model can be straightforwardly extended to describe three-component flows as follows.

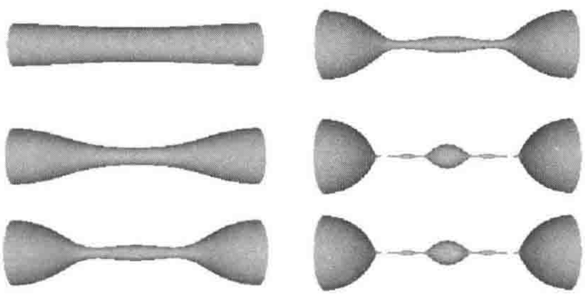


Figure 6 Time evolution leading to multiple pinch-offs. The evolution is from top to bottom and left to right. The domain is axisymmetric, the initial velocities are zero everywhere, and the concentration field is given by $c(r,z) = 0.5(1 - \tanh((r - 0.5 - 0.05\cos(z))/(2\sqrt{2}\epsilon)))$ on $\Omega = (0,\pi) \times (0,2\pi)$. Densities are matched and viscosity ratio is 0.5.

Consider a ternary mixture and denote the composition of components 1, 2, and 3, expressed as mass fractions, by c_1, c_2, and c_3, respectively. Therefore,

$$\sum_{i=1}^{3} c_i = 1, \quad 0 \le c_i \le 1 \qquad [24]$$

The composition of a ternary mixture (A, B, and C) can be mapped onto an equilateral triangle (the Gibbs triangle (Porter and Easterling 1993)) whose corners represent 100% concentration of A, B, or C as shown in **Figure 7a**. Mixtures with components lying on lines parallel to $\overline{BC}$ contain the same percentage of A, those with lines parallel to $\overline{AC}$ have the same percentage of B concentration, and analogously for the C concentration. In **Figure 7a**, the mixture at the position marked '∘' contains 60% A, 10% B, and 30% C. Because the concentrations sum to unity, only two of them need to be determined, say c_1, c_2.

The evolution of c_1 and c_2 is governed by the following advective ternary Cahn–Hilliard equation:

$$\frac{\partial c_1}{\partial t} + \boldsymbol{u} \cdot \nabla c_1 = \nabla \cdot (M(c_1, c_2) \nabla \mu_1) \qquad [25]$$

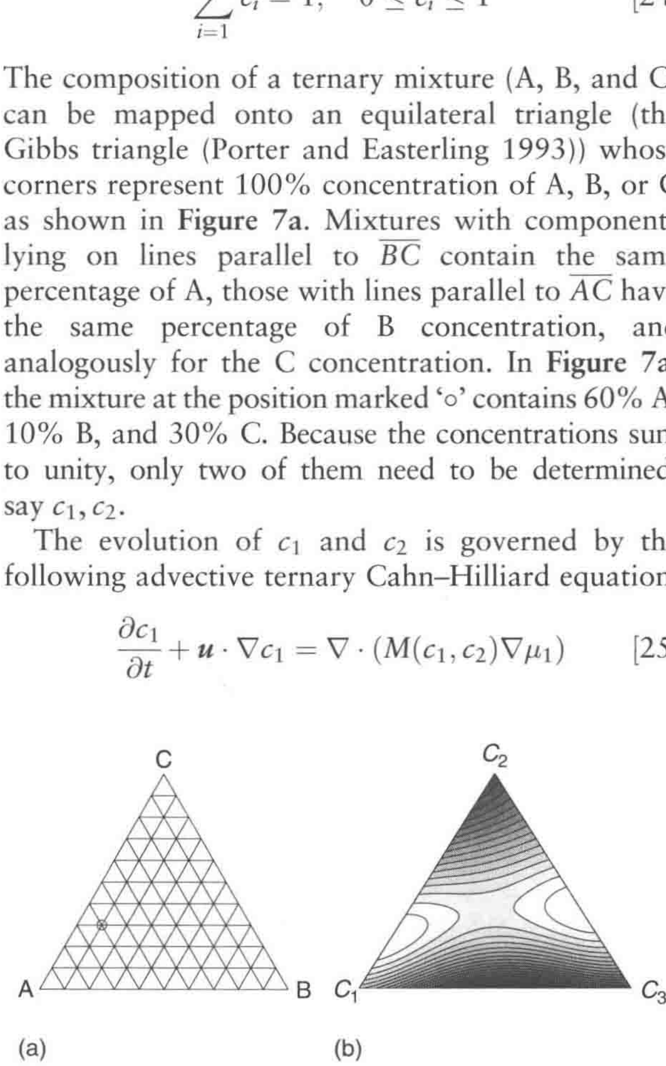


Figure 7 (a) Gibbs triangle. (b) Contour plot of the free energy $F(c_1, c_2)$ on the Gibbs triangle.

$$\frac{\partial c_2}{\partial t} + \boldsymbol{u} \cdot \nabla c_2 = \nabla \cdot (M(c_1, c_2)\nabla \mu_2) \quad [26]$$

$$\mu_1 = \frac{\partial F(c_1, c_2)}{\partial c_1} - \epsilon^2 \Delta c_1 - 0.5\epsilon^2 \Delta c_2 \quad [27]$$

$$\mu_2 = \frac{\partial F(c_1, c_2)}{\partial c_2} - 0.5\epsilon^2 \Delta c_1 - \epsilon^2 \Delta c_2 \quad [28]$$

where $M(c_1, c_2) = \sum_{i<j}^{3} c_i c_j$ is the mobility and $F(c_1, c_2)$ is the Helmholtz free energy that can be used to model the miscibility of the components. An example of a free energy (used in the simulation shown in **Figure 8** below) for which fluids 1 and 3 are immiscible and fluid 2 is preferentially miscible with fluid 3 is:

$$F(c_1, c_2) = 2c_1^2(1 - c_1 - c_2)^2 + (c_1 + 0.2)(c_2 - 0.2)^2 + (1.2 - c_1 - c_2)(c_2 - 0.4)^2$$

The contours of F on the Gibbs triangle are shown in **Figure 7b**.

The singular surface tension force is $F_{\text{sing}} = -6\sqrt{2}\epsilon \sum_{i=1}^{3} \tau_i \nabla \cdot (\nabla c_i \otimes \nabla c_i)$, where the physical surface tension coefficients τ_{ij} between two fluids i and j are decomposed into the phase-specific surface tensions τ_i such that $\tau_{ij} = \tau_i + \tau_j$.

As a demonstration of the evolution possible in partially miscible liquid systems, we present an example in which there is a gravity-driven (Rayleigh–Taylor) instability that enhances the transfer of a preferentially miscible contaminant from one immiscible fluid to another in 2D. In this system, the ternary Cahn–Hilliard system is solved using nonlinear multigrid methods and a projection method (Kim and Lowengrub (in press)) is used to solve the flow equations [5].

In **Figure 8** (first column), the top half of the domain initially consists of a mixture of fluids 1 and 2, and the bottom half consists of fluid 3, which is immiscible with fluid 1. The contours of c_1, c_2, and c_3 are visualized in gray-scale where darker regions denote larger values of c_1, c_2, and c_3, respectively. In the top row, the contours of fluid 1 are shown, the middle and bottom rows correspond to fluids 2 and 3, respectively.

Fluid 2 is preferentially miscible with fluid 3. Fluid 1 is assumed to be the lightest and fluid 2 the heaviest. The density of the 1/2 mixture is heavier than that of fluid 3, so the density gradient induces the Rayleigh–Taylor instability.

The evolution of the three phases is shown in **Figure 8**. As the simulation begins, the 1/2 mixture falls and fluid 2 diffuses into fluid 3. A characteristic Rayleigh–Taylor (inverted) mushroom forms, the

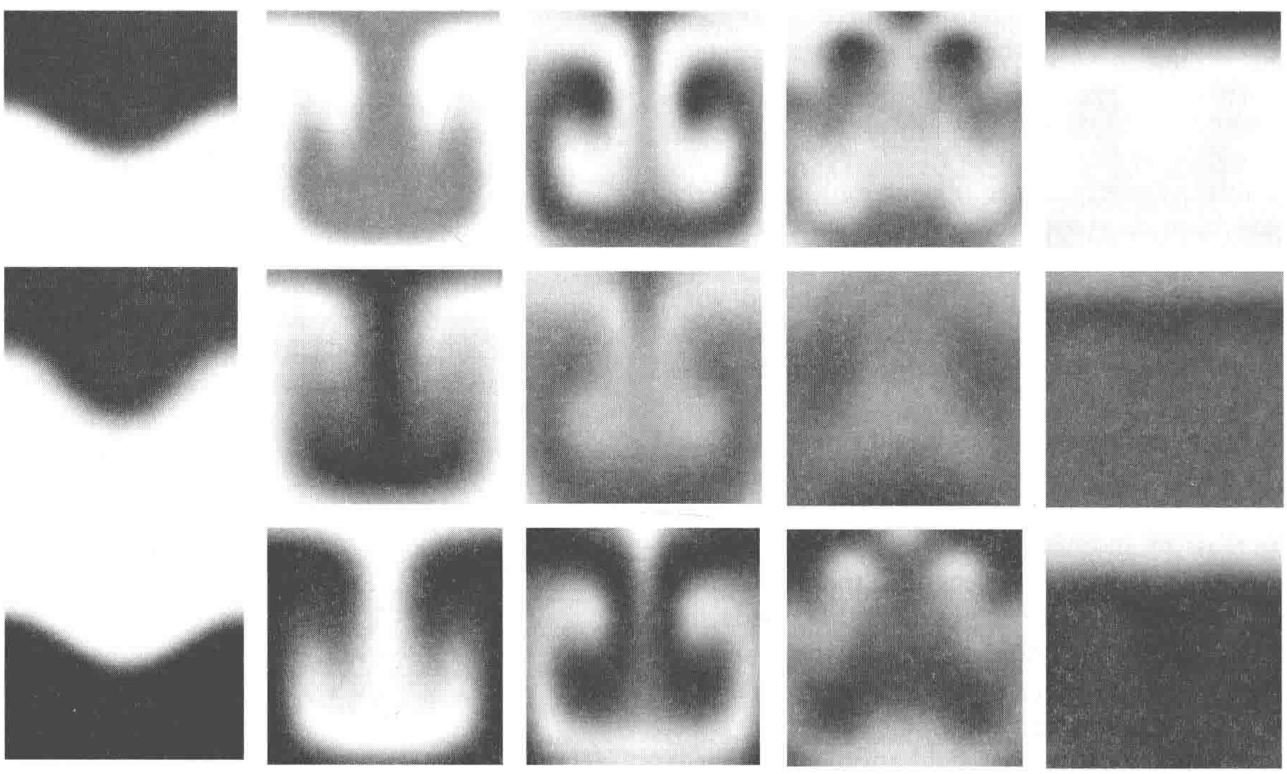


Figure 8 Evolution of concentration of fluid 1 (top row), 2 (middle row), and 3 (bottom row). The contours of c_1, c_2, and c_3 are visualized in gray-scale where darker regions denote larger values of c_1, c_2, and c_3, respectively.

surface area of the 1/3 interface increases, and vorticity is generated and shed into the bulk. As fluid 2 is diffused from fluid 1, the pure fluid 1 rises to the top as shown in **Figure 8**. Imagining that fluid 2 is a contaminant in fluid 1, this configuration provides an efficient means of cleansing fluid 1 since the buoyancy-driven flow enhances the diffusional transfer of fluid 2 from fluid 1 to fluid 3.

The advantages of the phase-field method are: (1) topology changes are automatically described; (2) the composition field c has a physical meaning not only near interface but also in the bulk phases; (3) complex physics can easily be incorporated into the framework, the methods can be straightforwardly extended to multicomponent systems, and miscible, immiscible, partially miscible, and lamellar phases can be modeled.

Associated with diffuse interfaces is a small scale ϵ, proportional to the width of the interface. In real physical systems describing immiscible fluids, ϵ can be vanishingly small. However, for numerical accuracy ϵ must be at least a few grid lengths in size. This can make computations expensive. One way of ameliorating this problem is to adaptively refine the grid only near the transition layer. Such methods are under development by various research groups.

Phase-field methods have been used to model viscoelastic flow, thermocapillary flow, spinodal decomposition, the mixing and interfacial stretching, in a shear flow, droplet breakup process, wave-breaking and sloshing, the fluid motion near a moving contact line, and the nucleation and annihilation of an equilibrium droplet (see the references in the review paper Anderson *et al.* (1998)).

Conclusions and Future Directions

In this paper we have reviewed the basic ideas of interface-tracking and interface-capturing methods that are critical in simulating the motion of interfaces in multicomponent fluid flows. The differences between these various formulations lie in the representation and the reconstruction of interfaces. The advantages and disadvantages of the algorithms have been discussed. While there has been much progress on the development of robust multifluid solvers, there is much more work to be done. Promising future directions for research include the incorporation of adaptive mesh refinement into the algorithms and the development of efficient hybrid schemes that combine the best features of individual methods.

See also: Breaking Water Waves; Capillary Surfaces; Fluid Mechanics: Numerical Methods; Incompressible Euler Equations: Mathematical Theory; Inviscid Flows; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Viscous Incompressible Fluids: Mathematical Theory; Vortex Dynamics.

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Intermittency in Turbulence

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Introduction

Intermittency has several meanings in turbulence. The oldest one, now most often labeled "external" or "large-scale" intermittency, refers to the coexistence of turbulent and laminar regions in inhomogeneous turbulent flows, such as in boundary layers or in free shear layers. In those cases, the interface between laminar irrotational flow and turbulent vortical fluid is typically sharp and corrugated. An observer sitting near the edge of the layer is immersed in turbulent fluid only part of the time.

The intermittency coefficient γ measures the fraction of turbulent fluid over the sampling universe over which the statistics are taken. For example, in a boundary layer such as that in **Figure 1**, the intermittency coefficient as a function of wall distance measures the fraction of turbulent fluid at a given distance from the wall. External intermittency is important in any attempt to model realistic turbulent flows, which are almost always inhomogeneous. Consider, for example, the classical homogeneous relation in eqn [1] between the mean kinetic energy K of the turbulent fluctuations and the energy dissipation rate ε:

$$\varepsilon = C\frac{K^{3/2}}{L} \qquad [1]$$

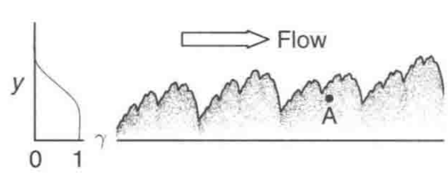


Figure 1 Sketch of a turbulent boundary layer, and of the associated intermittency factor. An observer such as A, at a distance y from the wall, only sees turbulent flow for a fraction γ of the time.

where L is the length scale of the largest eddies, and $C \approx 0.1$ is an experimentally determined constant. Such relations are often implicit in turbulent models, and they have to be modified to account for intermittency. Equation [1] only holds within the turbulent regions where the energy and the dissipation rates are K_T and ε_T, while the overall mean values used in the modeling conservation equations are $K = \gamma K_T$ and $\varepsilon = \gamma\varepsilon_T$. The true overall relation should therefore be

$$\varepsilon = C\gamma^{-1/2}\frac{K^{3/2}}{L} \qquad [2]$$

which may differ substantially from eqn [1], especially near the edge of the layer. Experimental values and rough theoretical estimates for the distribution of the intermittency coefficient are available for most practical turbulent flows.

Internal Intermittency

While the external intermittency just described is probably the most important one from the point of view of applications, it is not the most interesting from the theoretical point of view. Turbulence is a multiscale phenomenon which is inhomogeneous at all length scales, from the largest ones to the inner viscous cutoff (*see* Turbulence Theories). Moreover, this inhomogeneity goes beyond what could be expected just from the statistics of a random process. Consider, for example, the velocity difference Δu between two points separated by a distance r. The original Kolmogorov formulation of the energy cascade assumes that the probability density function (PDF), $p(\Delta u)$, is a universal function in the inertial range of scales, whose only parameter is a velocity scale depending on r. It then follows from Kolmogorov's analysis that

$$p(\Delta u) = F\left[\Delta u/(\bar{\varepsilon}r)^{1/3}\right] \qquad [3]$$

where $\bar{\varepsilon}$ is the average energy transfer rate across scales per unit mass, and the average $\overline{(\,)}$ is taken either over the whole flow or over a suitably designed ensemble of experiments. In an equilibrium system,

global energy conservation implies that $\bar{\varepsilon}$ is equal to the average viscous dissipation per unit mass:

$$\bar{\varepsilon} = \nu\overline{|\nabla \boldsymbol{u}|^2} \qquad [4]$$

In eqn [4], the kinematic viscosity of the fluid is ν, and $|\nabla \boldsymbol{u}|$ is the L_2-norm of the velocity gradient tensor. Equation [3] is valid as long as the separation r is much larger than the Kolmogorov viscous cutoff $\eta = (\nu^3/\bar{\varepsilon})^{1/4}$, and much smaller than the integral scale of the largest eddies $L_\varepsilon = u'^3/\bar{\varepsilon}$, where u' is the root-mean-square value of the fluctuations of one velocity component. The extent of this inertial range is a function of the Reynolds number $Re_L = u'L_\varepsilon/\nu$:

$$L_\varepsilon/\eta = Re_L^{3/4} \qquad [5]$$

The strict similarity hypothesis in eqn [3] is not well satisfied by experiments. While the velocity distribution at a given point is approximately Gaussian, **Figure 2a** shows that the velocity increments become increasingly non-Gaussian as the spatial separation is made much smaller than L_ε. It was also soon noted that the dependence of eqn [3] on a single parameter such as $\bar{\varepsilon}$ was theoretically suspect, since it is difficult to see how the PDFs of a whole set of local properties, such as the Δu for different intervals, could depend only on a single global property. Kolmogorov himself sought to bypass that difficulty by substituting eqn [3] by a "refined similarity" hypothesis,

$$p(\Delta u) = F\left[\Delta u/(\varepsilon_r r)^{1/3}\right] \qquad [6]$$

where ε_r is no longer a global average, but the mean value of the dissipation over a ball of radius of order r centered at the midpoint of the interval. This refined similarity is better satisfied by experiments (see **Figure 2b**), although, from the practical point of view, it just transfers the problem of characterizing Δu to that of characterizing the statistics of ε_r.

It has become customary to measure the behavior of $p(\Delta u)$ in terms of its structure functions,

$$S(n) = \int_{-\infty}^{\infty} \Delta u^n p(\Delta u)\mathrm{d}\Delta u \qquad [7]$$

which can be normalized as generalized flatness factors,

$$\sigma(n) = S(n)/S(2)^{n/2} \qquad [8]$$

It follows from the strict similarity hypothesis [3] that

$$S(n) \sim r^{n/3} \qquad [9]$$

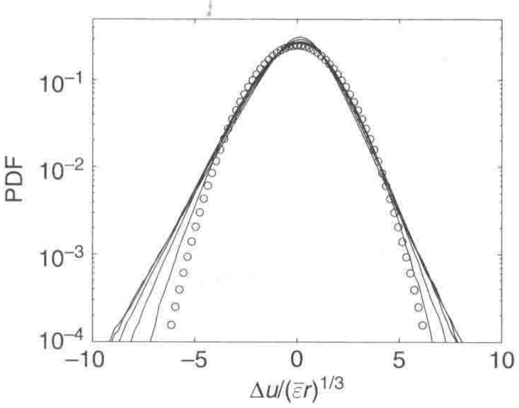
and that all the $\sigma(n)$ should be independent of the separation.

For example, the fourth-order flatness of a Gaussian distribution is $\sigma(4) = 3$. **Figure 3** shows that this is not true. The flatness increases as the separation decreases, and it only levels off at lengths of the order of the Kolmogorov viscous scale. For separations in that viscous range the flow is smooth, $\Delta u \approx (\partial_x u)r$, and

$$\sigma(n) \approx \overline{(\partial_x u)^n}/\overline{(\partial_x u)^2}^{n/2} \qquad [10]$$

It follows from eqn [10] and from **Figure 3** that the velocity gradients become increasingly non-Gaussian as L_ε and η separate at high Reynolds numbers. The velocity differences across intervals which are large with respect to η also become very non-Gaussian when $r \ll L_\varepsilon$.

Because the velocity difference between two points which are not too close to each other can be expressed as the sum of velocity differences over subintervals, a loose application of the central limit



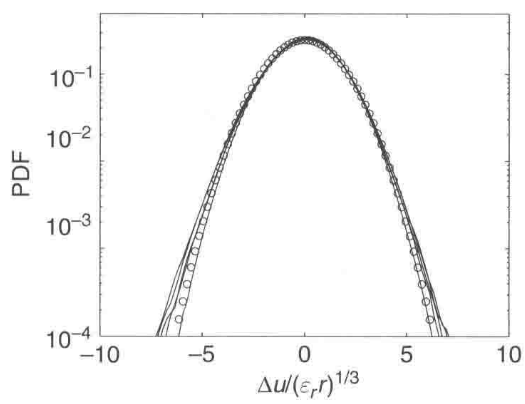


Figure 2 PDFs of the differences of the velocity component in the direction of the separation (for separations in the inertial range of scales). $r/L_\varepsilon = 0.02-0.36$, increasing by factors of 2; equivalent to $r/\eta = 180-3000$. Nominally isotropic turbulence at Reynolds number $Re_L = 10^5$.. (a) Δu is normalized with the global energy dissipation rate $\bar{\varepsilon}$; distributions are wider as the separation decreases. (b) Δu is scaled with the locally averaged dissipation over the separation interval. Data courtesy of H Willaime and P Tabeling.

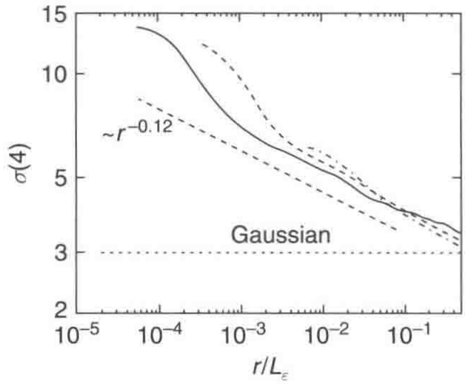


Figure 3 Fourth-order flatness of the differences of the velocity component in the direction of the separation, for separations in the inertial range of scales, $r/L_\varepsilon = 0.5$ to $r/\eta = 2$.. The Reynolds numbers of the different flows range from $Re_L = 1800$ to 10^6.. Data in part courtesy of H Willaime, P Tabeling, and R A Antonia.

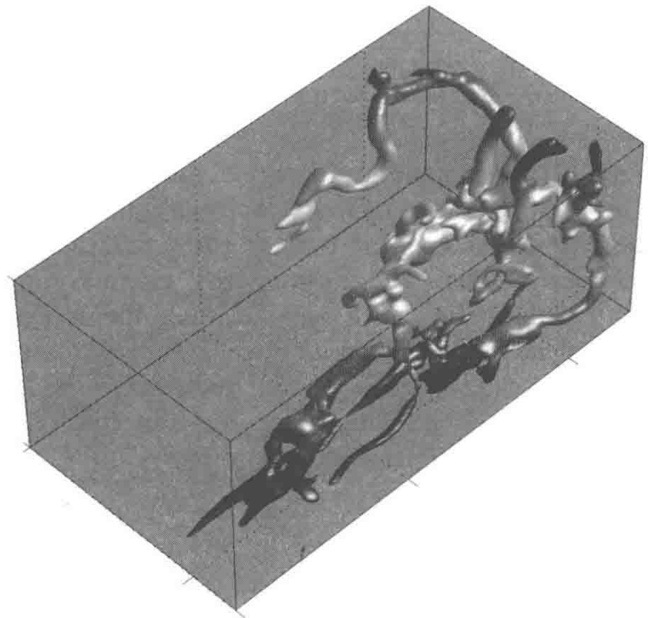


Figure 4 Intense vortex tangle in the logarithmic layer of a turbulent channel. The vortex diameters are of the order of 10η, and the size of the bounding box is of the order of the channel width. Reproduced with permission of J C del Álamo.

theorem would suggest that its PDF should be roughly Gaussian. The key conditions for that to happen are that the summands should be mutually independent, that their magnitudes should be comparable, and that each of them has a probability distribution with a finite variance. The first of those three conditions is probably a good approximation if the separation is much longer than the viscous cutoff, but the second one depends on the structure of the flow. The experimental non-Gaussian behavior suggests the existence of occasional very strong velocity jumps. In the viscous range of scales, those structures have been identified both experimentally and numerically as very strong linear vortices, in whose neighborhoods the strongest gradients are generated. An example of a tangle of such structures is shown in **Figure 4**.

In another example, the vorticity in decaying two-dimensional turbulence concentrates very quickly into relatively few strong compact vortices, which are stable except when they interact with each other. The velocity field is dominated by them, and the flatness of the velocity increments reaches values of the order of $\sigma(4) \approx 50$–100, even at moderate Reynolds numbers. That case is interesting because something can be said about the probability distribution of the velocity gradients. We have noted that the PDF of a sum of mutually comparable independent random variables with finite variances tends to Gaussian when the number of summands is large. This well-known theorem is a particular case of a more general result about sums of random variables whose incomplete second moments diverge as

$$\mu_2(s) = \int_{-s}^{s} x^2 p(x)\mathrm{d}x \sim s^{2-\alpha} \quad \text{when } s \to \infty \qquad [11]$$

When $0 < \alpha \leq 2$, the sums of such variables tend to a family of "stable" distributions parametrized by α. The Gaussian case is the limit of that family when $\alpha = 2$. In the case of two-dimensional vortices with very small cores, the velocity gradients at a distance R from the center of the vortex behave as $1/R^2$. If we take s in eqn [11] to be one of those velocity derivatives, its probability distribution is proportional to the area covered by gradients with a given magnitude, and

$$\mu_2(s) \sim \int_0^{s^{1/2}} R^{-4} 2\pi R\, \mathrm{d}R \sim s^{-1} \qquad [12]$$

The velocity derivatives at any point, which are the sums of the velocity derivatives induced by all the randomly distributed neighboring vortices, should therefore be distributed according to the stable distribution with $\alpha = 1$, which is Cauchy's

$$p(s) = \frac{c}{\pi(c^2 + s^2)} \qquad [13]$$

This distribution has no moments for $n > 1$. Its tails decay as s^{-2}, and the distribution of the gradients essentially reflects the properties of the closest vortex. In real two-dimensional turbulent flows, the distribution [13] is followed fairly well, but its extreme tails only reach to the maximum values of the velocity gradient found within the viscous vortex cores, which are not exactly point vortices.

Other similar general results can be derived that link the behavior of the structure functions with the properties of the stable distributions corresponding to the type of flow singularities expected in the limit of infinite Reynolds number.

The common feature of the two cases just described is the presence of strong structures that live for long times because viscosity stabilizes them. They are therefore more common than what could be expected on purely statistical grounds. They are responsible for the tails of the probability distributions of the velocity derivatives, but they are not the only intermittent features of turbulent flows. The increase of the flatness in **Figure 3** below $r \approx 50\eta$ is clearly connected with the presence of the coherent vortices, but even for larger separations there is a smooth evolution of $\sigma(4)$ that suggests that the formation of intense structures is a gradual process that takes place across the inertial range. Much less is known about those hypothetical inertial structures than about the viscous ones.

We can now recast the problem of intermittency in Navier–Stokes turbulence into geometric terms. The defining empirical observation for that system is that the energy dissipation given by eqn [4] does not vanish even in the infinite Reynolds number limit in which $\nu \to 0$. This means that the flow has to become singular as $\overline{|\nabla u|}L_\epsilon/u' \sim Re_L^{1/2}$. The strict similarity approximation assumes that those singularities are uniformly distributed across the flow, but the experimental evidence just discussed shows that this is not true. The singularities are distributed inhomogeneously, and the inhomogeneity develops across the inertial cascade. The problem of intermittency is to characterize the geometry of the support of the flow singularities in the limit of infinite Reynolds number.

In the absence of detailed physical mechanisms for the dynamics of the inertial range, most intermittency models are based on plausible processes compatible with the invariances of the inviscid Euler equations. The precise power law given in eqn [9] for the structure functions depends on the strict similarity hypothesis [3], but the fact that it is a power law only depends on the scaling invariances of the equations of motion. The energies and sizes of the eddies in the inertial range are too small for the integral scales of the flow to be relevant, and too large for the viscosity to be important. They therefore have no intrinsic velocity or length scales. Under those conditions, any function of the velocity which depends on a length has to be a power. Consider a quantity with dimensions of velocity, such as $u(r) = S(n)^{1/n}$, which is a function of a distance such as r. On dimensional grounds we should be able to write it as

$$u(r) = UF(\rho) \qquad [14]$$

where $\rho = r/L$, and L and $U(L)$ are arbitrary length and velocity scales. The value of $u(r)$ should not depend on the choice of units, and we can differentiate eqn [14] with respect to L to give

$$\partial_L u = (\mathrm{d}U/\mathrm{d}L)F(\rho) - U\rho L^{-1}(\mathrm{d}F/\mathrm{d}\rho) = 0 \qquad [15]$$

which can only be satisfied if

$$\frac{\mathrm{d}F}{\mathrm{d}\rho} = \zeta F \Rightarrow F \sim \rho^{\zeta} \qquad [16]$$

and $\zeta = L(\mathrm{d}U/\mathrm{d}L)/U$ is constant. This suggests generalizing eqn [9] to

$$S(n) \sim r^{\zeta(n)} \qquad [17]$$

where the exponents are empirically adjusted. Only $\zeta(3) = 1$ can be derived directly from the Navier–Stokes equations. Equation [17] implies that $\sigma(n)$ satisfies a power law with exponent $\zeta(n) - n\zeta(2)/2$. In **Figure 3**, for example, the flatness follows a reasonably good power law outside the viscous range, consistent with $\zeta(4) - 2\zeta(2) \approx -0.12$. The anomalous behavior near the viscous limit, and similar limitations at the largest scales, mean that only very high Reynolds number flows can be used to measure the scaling exponents, and that the range over which they are measured is never very large. Moreover, the integrand of the higher-order structure functions peaks at the extreme tails of the probability distributions of the velocity differences, which implies that very long experimental samples have to be used to accumulate enough statistics to measure the high-order exponents. For these and for other reasons, the scaling exponents above $n \gtrsim 8-10$ are poorly known. This is unfortunate because we will see later that some of the most interesting intermittency properties of the velocity field, such as the nature of the flow singularities in the infinite Reynolds number limit, depend on the behavior of the $\zeta(n)$ for large n.

Experimental values for the scaling exponents are given in **Table 1**. They are generally smaller than the ones predicted by the strict similarity approximation, implying that the moments of the velocity differences decrease with the separation more slowly than they would if they were self-similar, and suggesting that new stronger structures become important as the scale decreases.

Note that we have included in the table values for odd-order powers. Up to now we have not specified

Table 1 Longitudinal scaling exponents

Order	*Experimental*	*Strict similarity*
2	0..70 ± ..01	0.667
3	1.00	1
4	1..30 ± ..03	1.333
5	1..56 ± ..04	1.667
6	1..79 ± ..03	2.000
7	1..99 ± ..10	2.333
8	2..22 ± ..05	2.667

The values on the second column are averages from different experiments, and the standard deviations reflect scatter among experiments. The third column is the value from the strict similarity equation [9].

which velocity component is being analyzed, but most experiments refer to the one in the direction of the separation. That is the easiest case to measure, specially if time is used as a surrogate for distance, and those PDFs are not symmetric even in isotropic turbulence. Negative increments are more common than positive ones because of the extra energy required to stretch a vortex, and the effect is clearly visible in the distributions in **Figure 2**. Those longitudinal odd-order structure functions do not vanish, and their scaling exponents are the ones given in the table. The transverse structure functions are those in which the velocity component is normal to the separation, and their odd-order moments vanish by symmetry in isotropic turbulence. There has been a lot of discussion about whether the longitudinal scaling exponents of even orders differ from the transverse ones. Early results suggested that the latter are lower than the former, undermining the case for intermittency theories based on similarity arguments, and suggesting that a more mechanistic approach was needed. The present consensus seems to be that both sets of exponents are equal, but that there are residual effects of low Reynolds numbers and of flow anisotropy that are difficult to avoid experimentally. The question is still open.

Multiplicative Models

The most successful phenomenological models for the geometry of intermittency are based on the concept of a multiplicative cascade. Consider some flow property v, such as the locally averaged energy transfer rate by eddies of size r_k, which cascades into smaller eddies of size r_{k+1} which is some fraction of r_k. Denote by $p_k(v_k)$ the probability distribution of the value of v at the step k of the cascade.

Assume that the cascade is Markovian in the sense that the probability distribution of v_k depends only on its value in the previous step,

$$p_{k+1}(v_{k+1}) = \int p_{\mathrm{T}}(v_{k+1}|v_k;\, k)p_k(v_k)\,\mathrm{d}v_k \qquad [18]$$

This is in contrast to some more complicated functional dependence, such as on the values of v_k in some extended spatial neighborhood, or on several previous cascade stages. This assumption intuitively implies that v_{k+1} evolves faster, or on a smaller scale, than v_k, and that it is in some kind of equilibrium with its precursor. If the cascade is deterministic in that sense, v_k can be represented as a product

$$v_k/v_0 = q_k q_{k-1} \cdots q_1 \qquad [19]$$

in which the factors $q_k = v_k/v_{k-1}$ are statistically independent of each other.

If the underlying process is invariant to scaling transformations, the transition probability density function has to have the form

$$p_{\mathrm{T}}(v_{k+1}|v_k) = v_k^{-1} w(q_{k+1};\, k) \qquad [20]$$

The multiplicative model works most naturally for positive variables, and we will assume that to be the case in the following, but most results can be generalized to arbitrary distributions. We will also assume for simplicity that all the cascade steps are equivalent, so that the distribution $w(q)$ of the multiplicative factors is independent of k, and depends only on our choice for r_{k+1}/r_k.

Local deterministic self-similar cascades lead naturally to intermittent distributions, in the sense that the high-order flatness factors for v_k become arbitrarily large as k increases. It follows from eqns [18]–[20] that the nth order moment for p_k can be written as

$$S_k(n) = \int \xi^n p_k(\xi)\,\mathrm{d}\xi = S_0(n) S_w(n)^k \qquad [21]$$

where $S_w(n)$ is the nth order moment of the multiplicative factor q, and n is any real number for which the integral exists. If we define flatness factors as in eqn [7], we can rewrite eqn [21] as

$$\sigma_k(n) = \sigma_0(n)\sigma_w(n)^k \qquad [22]$$

It follows from Chebichev's inequality that

$$S(n) \geq S(n-2)S(2) \geq S(n-4)S(2)^2 \ldots \qquad [23]$$

from where

$$1 \leq \sigma(4) \leq \sigma(6) \ldots \qquad [24]$$

which is true for any distribution of positive numbers. Equality only holds for trivial distributions concentrated on a single value. The product in eqn [22] therefore increases without bound with the number of cascade steps, and the flatness factors diverge.

It is tempting to substitute k in [21] by a continuous variable, in which case the PDFs form a continuous semigroup generated by infinitesimal scaling steps. This leads to beautiful theoretical developments, but it is not necessarily a good idea from the physical point of view. For example, while it might be reasonable to assume that the properties of an eddy of size r depend only on those of the eddy of size $2r$ from which it derives, the same argument is weaker when applied to eddies of almost equal sizes. We will restrict ourselves here to the discrete case.

Limiting Distributions

The multiplicative process just described can be summarized as a family of distributions $p_k(v_k)$ such that the probability density for the product of two variables is

$$p(v_{k_1} v_{k_2}) = p_{k_1+k_2}(v_{k_1+k_2}) \qquad [25]$$

and it is natural to ask whether there is a limiting distribution for large k. We know that, in the case of sums, rather than products, such distributions tend to be Gaussian under fairly general conditions, and the first attempt to analyze [25] was to reduce it to a sum by defining

$$z = k^{-1} \log(v_k/v_0) \qquad [26]$$

The argument was that z would tend to a Gaussian distribution, and that the limiting distribution for v_k would be lognormal. This was soon shown to be incorrect. The central part of the distribution approaches lognormality, but the tails do not, because the central limit theorem says nothing about their behavior. The family of lognormal distributions is a fixed point of eqn [25], but it is unstable, and it is only attained if the individual generating distributions are themselves lognormal.

The lognormal distribution has moments

$$S_w(n) = \exp(an + bn^2) \qquad [27]$$

which are conserved under [21], so that the product of lognormally distributed variables stays lognormal. The moments in eqn [27] are generated by the recursive relation

$$Q_w(n) = \frac{S_w(n+3)S_w^3(n+1)}{S_w(n)S_w^3(n+2)} = 1 \qquad [28]$$

with suitable conditions for $n < 2$. Under [21], $Q_k(n) = Q_w^k(n)$, and it is clear that only when all the $Q_w(n)$ are exactly equal to 1 do they continue to be so under multiplication. Otherwise, any Q_w initially larger than 1 tends to infinity after enough cascade steps, while any one initially smaller than 1 tends to 0. Only an exactly lognormal distribution of the generating factors results in a lognormal limiting distribution, and even small errors lead to very different patterns of moments. This contrasts with the situation for sums of random variables, in which the Gaussian distribution is not only a fixed point, but also has a very large basin of attraction.

Multifractals

The problem with using the transformation [26] to find the limiting distribution of a multiplicative process is not so much the technique of analyzing the statistics of products in terms of those of sums, but the inappropriate use of the central limit theorem. It can be bypassed by using instead the theory of large deviations of sums of random variables. The key result is obtained by expanding the characteristic function of p_k when $k \gg 1$, and states that

$$p_k(v_k) \approx \left(\frac{-\phi_0''}{2\pi k}\right)^{1/2} e^{k[\phi(z)-z]} \qquad [29]$$

where z is defined as in [26] and ϕ, which plays the role of an entropy, is a smooth function of z. Primes stand for derivatives with respect to z. Let us define z_n as the point where

$$\phi_n' \equiv \phi'(z_n) = -n \qquad [30]$$

which corresponds to the location of the maximum of $\phi + nz$. The entropy ϕ can be computed from the moments of the transition probability density. Using Laplace's method to expand the nth moment of p_k, we obtain

$$S_k(n) = \int_{-\infty}^{\infty} k e^{k(n+1)z} p_k(v_k)\, dz \approx \left(\frac{\phi_0''}{\phi_n''}\right)^{1/2} e^{k(\phi_n + nz_n)} \qquad [31]$$

from where, using [21],

$$\lambda_n \equiv \log S_w(n) = \phi(z_n) + nz_n \qquad [32]$$

The essence of Laplace's approximation is that, for $k \gg 1$, most of the contribution to the integral in eqn [31] comes from the neighborhood of z_n, so that

it makes sense to consider each such neighborhood as a separate "component" of the cascade.

The geometric interpretation of this classification into components as a multifractal was developed in the context of three-dimensional homogeneous turbulence. We have up to now assumed very little about the nature of each cascade step, but it is natural in turbulence to interpret it as the process in which eddies decay to a smaller geometric scale. The argument works for any variable for which scale similarity can be invoked, but we have seen that most experiments are done for the magnitude of the velocity increments across a distance r. If we assume for simplicity that $r_k/r_{k+1} = \mathrm{e}$, so that $r_k/r_0 = \exp(-k)$, eqns [26] and [29] can be written as

$$v_k/v_0 = (r_k/r_0)^{-z_n}, \qquad p_k(z_n) \sim (r_k/r_0)^{-\phi_n} \qquad [33]$$

The multifractal interpretation is that the "component" indexed by n, whose velocity increments are "singular" in terms of r with exponent z_n, lies on a fractal whose volume is proportional to its probability, and which therefore has a dimension $D(z_n) = 3 + \phi_n$.

Note that eqn [32] implies that the scaling exponents in eqn [17] can now be expressed as

$$\zeta(n) = -\log S_w(n) = -\lambda_n \qquad [34]$$

There was an enumeration there of several things which are equivalent: the exponents, the spectra, the distribution, and the limiting distribution $p_\infty(v)$ – univocally determine each other. Note however that different quantities have different scaling exponents. For example, it follows from eqn [6] that, if the scaling exponents for the local dissipation are $\zeta_\varepsilon(n)$, the exponents for Δu would be $\zeta_{\Delta u}(n) = n/3 + \zeta_\varepsilon(n/3)$.

Some properties can be easily derived from the previous discussion. If we assume, for example, that the multiplicative factor q is bounded above by q_b, which is reasonable for many physical systems, eqn [26] implies that $z_n \leq \log q_\mathrm{b}$. In fact, if the transition probability behaves near q_b as $w(q) \sim (q_\mathrm{b} - q)^\beta$, the scaling exponents tend to

$$\lambda_n = n \log q_\mathrm{b} - (\beta + 1) \log n + \mathrm{O}(1) \qquad [35]$$

for $n \gg 1$. In the case in which $w(q)$ has a concentrated component at $q = q_\mathrm{b}$, the $\log n$ is missing in eqn [35]. In all cases, the singularity exponent of the set associated with $n \to \infty$ is $z_\infty = \log q_\mathrm{b}$, because the very high moments are dominated by the largest possible multiplier. In the case of a concentrated distribution the dimension of this set approaches a finite limit, but otherwise

$$D(n) \approx -(\beta + 1) \log n \qquad [36]$$

which becomes infinitely negative. This should not be considered a flaw. The set of events which only happen at isolated points and at isolated instants has dimension $D = -1$ in three-dimensional space, and those which only happen at isolated instants, and only under certain circumstances, have still lower negative dimensions. Sets with very negative dimensions are however extremely sparse, and are difficult to characterize experimentally.

The multifractal spectrum of the velocity differences in three-dimensional Navier–Stokes turbulence has been measured for several flows in terms of the scaling exponents, and appears to be universal. The probability distribution $w(q)$ of the multipliers has also been measured directly, and agrees well with the values implied by the exponents. It is also approximately independent of r, although not completely, perhaps due to the same experimental problems of anisotropy and limited Reynolds number which plague the measurement of the scaling exponents. There has been extensive theoretical work on the consequences of imposing various physical constraints on the multipliers, specially the conservation requirement that the average value of the dissipation has to be conserved across each cascade step. Several simple models have been proposed for the transition distribution which approximate the experimental exponents well, but the relation lacks specificity. Models that are very different give very similar results, and it is impossible to choose among them using the available data.

Multiplicative cascades and the resulting intermittency are not limited to Navier–Stokes turbulence. The equations of motion have only entered the discussion in this section through the assumption of scaling invariance. Multifractal models have in fact been proposed for many chaotic systems, from social sciences to economics, although the geometric interpretation is hard to justify in most of them. It is also important to realize that the fact that a given process can in principle be described as a cascade does not necessarily mean that such a description is a good one. Neither does a cascade imply a multiplicative process. For each particular case, we need to provide a dynamical mechanism that implements both the cascade and the transition multipliers. In three-dimensional Navier–Stokes turbulence, the basic transport of energy to smaller scales and to higher gradients is vortex stretching. The differential strengthening and weakening of the vorticity under axial stretching and compression also provide a natural way of introducing the self-similar transition probabilities of the local dissipation.

Examples of nonintermittent cascades abound. We have already mentioned that the vorticity in

decaying two-dimensional turbulence gets concentrated into stable vortex cores which eventually block the decay. The resulting enstrophy distribution is highly intermittent, but it is not well described by a multifractal. Conversely, forced two-dimensional turbulence is dominated by an inverse energy cascade to larger scales, which is not intermittent.

In addition, the intermittency of some systems is not a small-scale effect. Turbulent mixing of a passive scalar, which is the key process in turbulent heat transfer and in the atmospheric dispersion of pollutants, is an extremely intermittent phenomenon. The gradients of the scalar tend to be very localized, but they concentrate in sheets, narrow in thickness but otherwise extended. Some progress has recently been made on a simplified model due to Kraichnan for this problem, which is the linear stirring of a passive scalar by a random noise with delta correlation. Its statistics have been computed analytically, but the constraints of linearity and of uncorrelated forcing are strong, and the same methods do not appear to be extensible to mixing by real turbulence (*see* Lagrangian Dispersion (Passive Scalar)). Another problem in which intermittency is confined to large-scale surfaces is the motion of a three-dimensional pressureless gas, which has been used as a model for hypersonic turbulence and for the large-scale evolution of dark matter in the early universe.

In summary, intermittency is a fascinating property of many random systems, including three-dimensional Navier–Stokes turbulence, which interferes, sometimes strongly, with their description by simple cascade models. Significant advances have been made in its quantitative kinematic analysis. In some cases we also have a qualitative understanding of its roots. But in very few cases do we understand it well enough to make quantitative predictions.

See also: Ergodic Theory; Incompressible Euler Equations: Mathematical Theory; Lagrangian Dispersion (Passive Scalar); Turbulence Theories; Vortex Dynamics; Wavelets: Applications.

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Intersection Theory

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Introduction

Intersection theory is the theory that governs the rigorous definition of intersections of cycles. This can take place in a variety of mathematical contexts, for instance, the intersections of two cycles on an oriented manifold in algebraic topology, of two currents on a differentiable manifold in differential geometry, or of two subvarieties on a nonsingular algebraic variety in algebraic geometry.

In algebraic geometry the theory is especially well developed (Fulton 1998). A cycle on an algebraic variety (or scheme) is a formal linear combination of irreducible closed subvarieties. These are subject to an equivalence relation called rational equivalence. For every rational function on every subvariety, its zero set is deemed rationally equivalent to its poles (with appropriate multiplicities).

As an example, in the complex projective plane $\mathbb{CP}^2$, any two lines are rationally equivalent since the ratio of two linear forms will vanish on one line and have a pole along the other. Similarly, a curve of degree d is rationally equivalent to d lines. Any two points in $\mathbb{CP}^2$ can be joined by a line (a copy of

$\mathbb{CP}^1$), and a rational function on $\mathbb{CP}^1$ can be chosen to vanish at one point and have a pole at the other. The groups of cycles modulo rational equivalence, known as Chow groups, are

$$CH_2(\mathbb{CP}^2) \cong \mathbb{Z}, \quad \text{generated by the fundamental class } [\mathbb{CP}^2]$$
$$CH_1(\mathbb{CP}^2) \cong \mathbb{Z}, \quad \text{generated by the class of a line}$$
$$CH_0(\mathbb{CP}^2) \cong \mathbb{Z}, \quad \text{generated by the class of a point}$$

Two distinct lines ℓ_1 and ℓ_2 meeting at a point p have this point as their intersection-theoretic product:

$$[\ell_1] \cdot [\ell_2] = [p] \qquad [1]$$

Intersection theory must also provide a self-intersection $[\ell_1] \cdot [\ell_1]$. Because ℓ_1 and ℓ_2 are rationally equivalent, this must also be the class of a point, but symmetry precludes the choice of a distinguished point on ℓ_1. Instead, $[\ell_1] \cdot [\ell_1]$ is declared to be the rational equivalence class of a point on ℓ_1, an element of $CH_0(\ell_1)$ rather than a specific cycle. This example illustrates that intersections cannot generally be defined on the level of cycles.

Algebraic Intersection Products

Refined Intersections

For a general nonsingular variety X, say of dimension m, if U and V are subvarieties of X of respective dimensions c and d, then there is a refined intersection product

$$[U] \cdot [V] \in CH_{c+d-m}(U \cap V) \qquad [2]$$

The traditional definition of the intersection product is based on two ideas. First, given two cycles that intersect properly, which by definition means that no component of their intersection has codimension less than the sum of the codimensions of the given cycles, the intersection product should be a formal sum of these components, each with a multiplicity that correctly reflects the geometry of the intersection. Second, given two arbitrary cycles, it should be possible to replace one of them by a rationally equivalent cycle which intersects the other properly.

While these ideas are simple, it took several decades for them to be carried out successfully. The case of curves on a surface meeting at a point was understood in the nineteenth century. Generalizing the classically understood canonical divisor class on a variety, work in the 1930s by Severi, Todd, and others showed that there are groups of equivalence classes of cycles in which canonical invariants of higher degrees can be defined (in modern language, higher Chern classes of the tangent bundle). Weil's foundations for algebraic geometry of the 1940s included a study of intersections of cycles. It was not until the 1950s that the notion of Chow groups was formalized and intersection theory was properly developed in this context. Chevalley, Chow, Samuel, Severi, and others contributed essential components of the theory. In an interesting parallel development, an intersection theory based on intersection multiplicities in algebraic topology was put forth by Alexander and Lefschetz in the 1920s, a decade before the introduction of the cup product in cohomology.

Deformation to the Normal Cone

In the 1970s, Fulton and MacPherson established a construction of the intersection product in algebraic intersection theory that does not require moving cycles into general position. To accomplish this, they used an elegant geometric construction known as deformation to the normal cone.

Let $i: X \to Y$ be an embedding of codimension d of nonsingular varieties. Let V be a subvariety of Y of dimension k whose intersection with X is of interest. We may view X as the zero set of a section s of some algebraic vector bundle E on Y. By

$$(y, \lambda) \mapsto (\lambda^{-1}s(y), \lambda)$$

we have a map of the product of Y with the punctured affine line, $Y \times (\mathbb{A}^1 \setminus \{0\})$, into $E \times \mathbb{A}^1$. We denote the closure of the image by $M_X^\circ Y$. An alternative, more intrinsic description is in terms of the blowup construction of algebraic geometry:

$$M_X^\circ Y = Bl_{X \times \{0\}}(Y \times \mathbb{A}^1)$$

Geometrically, $M_X^\circ Y$ has a copy of Y over each $\lambda \neq 0$ and a copy of the normal bundle $N_X Y$ over $\lambda = 0$. This is the key construction that Fulton and MacPherson make use of. The same construction applied to V, that is, the closure of $V \times (\mathbb{A}^1 \setminus \{0\})$ in $M_X^\circ Y$, has over 0 a sort of singular normal bundle known as the normal cone

$$C_{X \cap V} V \subset N_X Y|_{X \cap V}$$

One of the properties of Chow groups is that they are unchanged upon pullback to the total space of a vector bundle (apart from the obvious dimension shift). The refined intersection of V with X, denoted $i^![V]$, is defined to be the unique element of $CH_{k-d}(X \cap V)$ whose pullback to $N_X Y$ is equal to $[C_{X \cap V} V]$.

This single construction encompasses and interpolates between two extreme cases of intersections:

$$i^![V] = [X \cap V] \quad \text{when } X \text{ and } V \text{ meet transversely} \qquad [3]$$

$$i^![V] = c_d(N_X Y) \cap [V] \quad \text{when } V \subset X \qquad [4]$$

Equation [3] makes reference to transverse intersection, a notion that is stronger than proper intersection. In situations when it applies, for example, in eqn [1], it signifies that intersection operations behave as one might expect. Equation [4] includes the self-intersection formula which says that $[X] \cdot [X]$ is equal to the top Chern class of $N_X Y$.

With this construction, which is well documented in Fulton (1998), the general refined intersection in eqn [2] is obtained by reduction to the diagonal. Let Δ_X denote the diagonal inclusion $X \to X \times X$ of the nonsingular variety X. For subvarieties U and V of X, we define

$$[U] \cdot [V] = \Delta_X^![U \times V] \qquad [5]$$

Equation [5] makes the Chow groups of X into a ring, the Chow ring $CH^*(X)$, which is graded by codimension by setting

$$CH^k(X) = CH_{m-k}(X)$$

Links with Topology

Cycle Map to Homology

For algebraic varieties over the complex numbers, there is a cycle map which links the Chow groups with a topological homology group. If X is an algebraic variety over $\mathbb{C}$, then let $H_*(X)$ denote the Borel–Moore homology of X, that is, the homology of locally finite singular chains on X (viewed as a topological space with the classical topology). If X is embedded as a closed subset of an oriented differentiable manifold M, then there are identifications

$$H_i(X) \cong H^{n-i}(M, M \setminus X) \qquad [6]$$

where n is the dimension of M. There is a cycle class map

$$CH_k(X) \to H_{2k}(X)$$

which sends the class of each irreducible subvariety Z of dimension k in X to its fundamental class $[Z] \in H_{2k}(X)$.

Let M be an oriented differentiable manifold of dimension n and let X and Y be closed subsets of M. Then the cup product $H^i(M, M\setminus X) \otimes H^j(M, M\setminus Y) \to H^{i+j}(M, M\setminus(X \cap Y))$ induces, via eqn [6], an intersection product

$$H_i(X) \otimes H_j(Y) \to H_{i+j-n}(X \cap Y)$$

which is the topological analog of the refined intersection product of eqn [5]. The products are compatible via the cycle class map. The topology of complex algebraic varieties and the compatibilities between algebraic and topological intersections are discussed in Fulton (1998). An interesting application of this interplay of intersection theories is the convolution product in Borel–Moore homology, which is important in geometric representation theory (see Chriss and Ginzburg (1997)).

Riemann–Roch Theorems

The classical Riemann–Roch theorem relates the dimensions of linear systems on an algebraic curve (algebraic quantities) with their degrees and the curve's genus (topological quantities). The Hirzebruch–Riemann–Roch theorem states that on a nonsingular projective variety X, if E is an algebraic vector bundle on X and $\chi(E)$ denotes its Euler characteristic (the alternating sum of the ranks of the sheaf-theoretic cohomology groups), then

$$\chi(E) = \int_X \mathrm{ch}(E) \cdot \mathrm{td}(T_X) \qquad [7]$$

where $\int_X$ denotes the degree of the zero-dimensional component of the quantity that follows, and the Chern character $\mathrm{ch}(E)$ and Todd class $\mathrm{td}(T_X)$ are certain standard universal polynomials of Chern classes.

Grothendieck had the inspired idea that eqn [7] could be generalized to a covariance property for the Chern character times the Todd class. If X and Y are nonsingular varieties and $f: X \to Y$ is a projective morphism (or, more generally, a proper morphism), then there is a well-defined push-forward f_* on Chow groups. There is also a kind of push-forward for vector bundles. The Grothendieck group of vector bundles on X, denoted $K^0(X)$, is the group of formal linear combinations of vector bundles, modulo the relations $[E] = [E'] + [E'']$ whenever E' is a sub-bundle of E with quotient bundle E''. Every coherent sheaf $\mathcal{F}$ has a well-defined class in $K^0(X)$, namely, the alternating sum of $[E_i]$ where $E_\bullet$ is any finite resolution of $\mathcal{F}$ by vector bundles (locally free sheaves). The push-forward $f_*[E]$ is defined as the alternating sum of the classes in $K^0(Y)$ of the higher direct images $R^i f_* E$. The Grothendieck–Riemann–Roch theorem states that

$$\mathrm{ch}(f_*[E]) \cdot \mathrm{td}(T_Y) = f_*(\mathrm{ch}(E) \cdot \mathrm{td}(T_X)) \qquad [8]$$

in $CH_*(Y) \otimes \mathbb{Q}$. Notice that eqn [7] represents the case that Y is a point.

There is an even more general formulation valid for singular varieties. It is necessary to work with a homology version of the Grothendieck group, namely, the Grothendieck group $K_0(X)$ of coherent sheaves on X. The Baum–Fulton–MacPherson version of the Grothendieck–Riemann–Roch theorem prescribes transformations

$$\tau_X : K_0(X) \to CH_*(X) \otimes \mathbb{Q} \quad [9]$$

which are covariant for proper morphisms. When X is nonsingular, τ_X is given by the "Chern character" times the "Todd class", and covariance becomes eqn [8].

In the case of varieties over the complex numbers, there is also a transformation from the algebraic Grothendieck group $K_0(X)$ to a topological analog, satisfying various compatibilities. The composition with the homology Chern character gives Riemann–Roch transformations $K_0(X) \to H_*(X; \mathbb{Q})$ satisfying properties akin to those of eqn [9].

The Analytic Setting

The Atiyah–Singer index theorem stands as an important generalization of the Hirzebruch–Riemann–Roch theorem. The index of an elliptic differential operator on a differentiable manifold plays the role of the Euler characteristic, and is equated with a topological quantity. One of the consequences of the index theorem is the validity of eqn [7] for general compact complex manifolds.

More in the domain of pure analysis is the question of intersecting two currents on a differentiable manifold. Currents arise naturally out of Chern–Weil theory. To each current is associated a wave front, a subset of the cotangent bundle that reflects the geometry of the singular set of the current. A current can be pulled back to an embedded submanifold whenever the embedding is transverse to the wave front. By reduction to the diagonal, this gives an intersection of two currents with transverse wave fronts which reduces to the usual wedge product in the case of smooth differential forms (see Hörmander (1990)).

Applications of Intersection Theory

Enumerative Geometry

Intersection theory has proved to be a useful tool in diverse areas such as enumerative geometry, singularity theory, and moduli problems. Enumerative problems have intrigued generations of geometers. Chasles, Maillard, Schubert, and Zeuthen are among the geometers of the second half of the nineteenth century who solved an impressive array of problems, including, as a notable example, Steiner's five conics problem to determine the number of plane conics tangent to five given conics in general position.

In modern terms, the successful solution to an enumerative problem involves setting up a space which parametrizes the geometric objects being counted, suitably compactified, and carrying out an intersection-theoretic computation on this space. Steiner's problem illustrates how "excess intersection" can occur and cause difficulty. Inside the $\mathbb{CP}^5$ of plane conics, including degenerate conics, those tangent to a given conic constitute a sextic hypersurface. So $6^5 = 7776$ would appear plausible; this was, in fact, the originally proposed solution. However, the most degenerate conics, the double lines, all appear as limits of families of conics tangent to any given conic. The refined intersection of five of these sextics has a cycle class of degree 4512 supported on the Veronese surface of double lines. This leaves 3264, the correct answer given by Chasles in 1864. The issue of providing rigorous foundations for these kinds of calculations was recognized by Hilbert, who set it as the 15th of his 23 major mathematical problems outlined in 1900. A good survey of early and modern efforts in enumerative geometry can be found in Kleiman and Thorup (1987).

Singularity Theory and Degeneracy Loci

In any situation where a geometric object is described by parameters, there will be values of the parameter at which the geometry changes qualitatively. The significance of this is evident in the space of conics above. Singularity theory is concerned with the loci in parameter spaces on which these transitions can occur. Let $\pi : Y \to P$ be a map of differential manifolds, or of nonsingular algebraic varieties, which is generally (but not everywhere) submersive, so that there are singular fibers. Let d denote the dimension of P, which can be considered as a parameter space, and let c be the dimension of Y. Consider the loci

$$\bar{S}_k(\pi) = \{y \in Y \mid \mathrm{rk}(T_{y,Y} \to T_{\pi(y),P}) \le d - k\}$$

of singularity theory. Thom made an influential study of these in the 1950s, and Porteous in 1971 gave the following formula, now called the Thom–Porteous formula:

$$[\bar{S}_k(\pi)] = s_{((k+c-d)^k)}(\pi^* T_P - T_Y) \quad [10]$$

The symbol on the right is shorthand for $s_{(k+c-d,\dots,k+c-d)}$, the case $a_1 = \cdots = a_k = k + c - d$ of the Schur determinant $s_{(a_1,\dots,a_k)} = \det(s_{a_i+j-i})_{1\le i,j\le k}$, and for vector bundles E and F the $s_i(F - E)$ are

defined by the formula $s(F - E) = \sum_i (-1)^i c_i(E) / \sum_i (-1)^i c_i(F)$. In algebraic intersection theory, eqn [10] has the precise meaning that when $\bar{S}_k(\pi)$ has the expected codimension $k(k + c - d)$ in Y (or is empty), its cycle class is equal to the given polynomial in Chern classes. The Thom–Porteous formula applies to the degeneracy loci of arbitrary maps of vector bundles $E \to F$. Degeneracy loci constitute an active area of research in intersection theory, and there are generalizations, for example, to cases where there are more bundles or bundle maps with symmetry (see Fulton and Pragacz (1998)).

Moduli Spaces

The parameter spaces that have appeared often admit interpretations as moduli spaces. Moduli problems start with geometric objects to be classified, and ask for families of these objects over an arbitrary base space to be represented as faithfully as possible by maps from the base space to some space called a moduli space. For enumerative applications it is most useful for the moduli space to be compact. One of the principal examples is the moduli of algebraic curves of given genus g: for $g \geq 2$, the moduli space of smooth curves M_g has a compactification $\bar{M}_g$ by stable curves, as defined and studied by Deligne and Mumford. While the M_g are singular, the singularities are mild enough to permit the definition of an intersection theory for M_g and $\bar{M}_g$, as was done by Mumford in the 1980s. More generally, if X is a complex projective variety, Kontsevich's spaces of stable maps $\bar{M}_{g,n}(X, \beta)$ compactify the moduli of genus g curves with n marked points together with algebraic maps to X having image in homology class $\beta \in H_2(X)$. These spaces, and some high-powered intersection theory that takes place on them, are vitally important in Gromov–Witten theory. K-theory also provides an alternative approach to intersection products in algebraic geometry.

Extensions and Related Theories

Motives and Higher Chow Groups

Intersection theory has evolved into a mature theory with numerous extensions and offshoots. Many of these are a result of endeavors to forge links with other branches of mathematics. One of the extensions, higher Chow groups, has its roots in a basic property of intersection theory, the excision property, which states that if X is a variety and $U \subset X$ an open subvariety, with $Z = X \setminus U$, then the inclusion and restriction maps fit into a right exact sequence

$$CH_*Z \to CH_*X \to CH_*U \to 0$$

This is reminiscent of the long exact homology sequence of a pair in algebraic topology. Indeed, there is a corresponding long exact sequence of Borel–Moore homology groups, but the elementary algebraic theory lacks such a long exact sequence. Bloch introduced higher Chow groups in the 1980s to fill this gap. The theory, which is quite complicated, provides groups $CH_*(X, j)$, with $CH_*(X, 0) = CH_*X$, such that there is a long exact sequence

$$\cdots \to CH_*(U, j+1) \to CH_*(Z, j) \to CH_*(X, j) \to CH_*(U, j) \to \cdots$$

These groups are closely connected to algebraic K-theory and also to a related theory called motivic cohomology.

Motives, a sort of universal cohomology theory envisaged by Grothendieck, conjecturally form a category which can be extended to a bigger category of mixed motives that reflects mixed structures in cohomology, such as mixed Hodge structures. Recently, Voevodsky *et al.* (2000) have introduced motivic cohomology groups which form an integral part of a homotopy theory for algebraic varieties. Voevodsky's work, including a proof of the Milnor conjecture of K-theory, earned him a Fields Medal in 2002.

Arithmetic Intersection Theory

There is an arithmetic version of intersection theory which applies to an arithmetic scheme X, which is, informally, a scheme defined over every prime field (all finite fields $\mathbb{F}_p$ and also $\mathbb{Q}$) in a consistent way. This means that X can be base-extended to any field. In situations where the complex variety $X(\mathbb{C})$ is nonsingular, there is an arithmetic Chow ring $\widehat{CH}^*(X)$, introduced by Gillet and Soulé in 1990. Elements of $\widehat{CH}^*(X)$ are equivalence classes of pairs (Z, g) where Z is an algebraic cycle on X and g is known as a Green current for Z, a current on $X(\mathbb{C})$ satisfying the relation

$$\frac{\mathrm{i}}{2\pi}\partial\bar{\partial}g + \delta_{Z(\mathbb{C})} = \omega \qquad [11]$$

for some smooth differential form ω satisfying some conditions. Here, $\delta_Z(\mathbb{C})$ denotes the current of integration along $Z(\mathbb{C})$. The point to notice is that eqn [11] relates analysis (the Green current) and algebra (the cycle) on X on one side with topology on the other, as ω will be a closed form whose class in de Rham cohomology is Poincaré dual to $[Z(\mathbb{C})]$.

Arithmetic intersection theory is used to define arithmetic height functions. Height functions have important applications to Diophantine problems, and were an essential component of the proof by Faltings of the Mordell conjecture, which earned him a Fields Medal in 1986. Arithmetic intersection theory grew

out of an earlier theory of Arakelov, in which $X(\mathbb{C})$ is endowed with a Kähler metric, and the form ω in eqn [11] is required to be harmonic. The Arakelov Chow group is only a ring when harmonic forms are closed under wedge product, which is not the case generally but which is true in some interesting cases, for example, for Grassmannian varieties. Arakelov treated the case of arithmetic surfaces, that is, the case when $X(\mathbb{C})$ is an algebraic curve ("surface" refers to a second dimension in the arithmetic direction), and introduced a pairing of arithmetic divisors, in analogy with the usual pairing of divisors on an algebraic surface. Arakelov's work, its subsequent generalizations, and more recent developments are covered in Faltings (1992).

Equivariant Theories and Stacks

Moduli problems such as those mentioned previously are often best represented not by traditional varieties, but by a more sophisticated sort of object called a stack. Taking inspiration from Mumford's intersection theory on M_g, intersection theory on algebraic stacks has grown into a mature theory in its own right. Examples of stacks include orbifolds, for which there is the Chen–Ruan (orbifold) cohomology theory as well as an algebraic analog due to Abramovich, Graber, and Vistoli (see Abramovich, *et al.* (2002)). Another class of examples are quotient stacks of a variety by the action of an algebraic group. In these cases the Chow groups of the stack are equivariant Chow groups, part of a rich theory modeled on equivariant cohomology in algebraic topology. Behrend (2002) provides a nice survey of stacks, equivariant intersection theory, and their uses in Gromov–Witten theory. The Bott residue formula is an important tool in equivariant intersection theory which is particularly well suited to making concrete calculations, for example, in enumerative geometry. A description with nice examples can be found in Ellingsrud and Strømme (1996).

See also: Cohomology Theories; Hamiltonian Group Actions; Index Theorems; *K*-Theory; Moduli Spaces: An Introduction.

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Inverse Problem in Classical Mechanics

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Formulation of the Problem

Consider the Newton equation

$$\ddot{x} = F(x), \quad F(x) = -\nabla v(x), \qquad x \in \mathbb{R}^d \qquad [1]$$

where

$$v \in C^2(\mathbb{R}^d, \mathbb{R})$$
$$|\partial_x^j v(x)| \le c_{|j|}(1+|x|)^{-\alpha-|j|} \qquad [2]$$
$$\text{for } x \in \mathbb{R}^d, |j| \le 2, \text{and some } \alpha > 1, c_{|j|} \ge 0$$

(where j is the multi-index $j \in (\mathbb{N} \cup \{0\})^d$, $|j| = \sum_{n=1}^d j_n$). In classical mechanics, eqn [1] describes the dynamics of a particle with the mass $m = 1$ in the force field F with the potential v. For eqn [1] the energy $E = (1/2)(\dot{x}(t))^2 + v(x(t))$ is an integral of motion.

Under the assumptions [2], it follows that (Reed and Simon 1979): for any $(p_-, x_-) \in \mathbb{R}^{2d}, p_- \neq 0$, eqn [1] has a unique solution $x \in C^2(\mathbb{R}, \mathbb{R}^2)$ such that

$$\begin{aligned} &x(t) = p_- t + x_- + y_-(t) \\ &y_-(t) \to 0, \quad \dot{y}_-(t) \to 0, \qquad \text{as } t \to -\infty \end{aligned} \qquad [3]$$

in addition, for almost any (p_-, x_-)

$$x(t) = a(p_-, x_-)t + b(p_-, x_-) + y_+(t)$$
$$a(p_-, x_-) \neq 0, \ y_+(t) \to 0, \ \dot{y}_+(t) \to 0 \quad \text{as } t \to +\infty \qquad [4]$$

furthermore, the set $\mathcal{D}$ of all $(p_-, x_-) \in \mathbb{R}^{2d}, p_- \neq 0$, for which [4] holds for fixed v, is an open subset of $\mathbb{R}^{2d}$ and $\mathcal{M}es(\mathbb{R}^{2d} \backslash \mathcal{D}) = 0$.

We say that a, b arising in [4] (and defined on $\mathcal{D}$) are the scattering data for eqn [1]. In addition, the scattering data a, b at fixed energy $E > 0$ means a, b on $\{(p_-, x_-) \in \mathcal{D} \,|\, p_-^2/2 = E\}$. Roughly speaking, for a particle moving according to [1], the functions a, b relate the free motion at time $t \to -\infty$ with the free motion at time $t \to +\infty$.

Note that

$$a(p_-, x_- + t_0 p_-) = a(p_-, x_-)$$
$$b(p_-, x_- + t_0 p_-) = b(p_-, x_-) + t_0 a(p_-, x_-) \qquad [5]$$
$$(p_-, x_-) \in \mathcal{D}, \quad t_0 \in \mathbb{R}$$

Formula [5] imply that a, b on $\mathcal{D}$ are uniquely determined by a, b on $\{(p_-, x_-) \in \mathcal{D} \,|\, p_- x_- = 0\}$, where $p_- x_-$ is the scalar product of p_- and x_-.

If $v(x) \equiv 0$, then $a(p_-, x_-) = p_-, b(p_-, x_-) = x_-, (p_-, x_-) \in \mathbb{R}^d, p_- \neq 0$. Therefore, it is convenient to use for a, b the following representation:

$$a(p_-, x_-) = p_- + a_{sc}(p_-, x_-)$$
$$b(p_-, x_-) = x_- + b_{sc}(p_-, x_-), \quad (p_-, x_-) \in \mathcal{D} \qquad [6]$$

where the subscript sc is an abbreviation of the word "scattering."

The direct scattering problem for eqn [1], under the assumptions [2], consists in the following: given v, find a, b.

The inverse-scattering problem for eqn [1], under the assumptions [2], consists in the following: given a, b (or some partial information about a, b), find v.

In the present article, we discuss, mainly, the aforementioned inverse-scattering problem.

Abel's Result of 1826

Consider the Newton equation [1] in dimension $d = 1$ for $x \in]-\infty, x_1], x_1 > 0$, where

$$v \in C^2(]-\infty, x_1], \mathbb{R})$$
$$v(x) = 0 \quad \text{for } x < 0 \qquad [7]$$
$$\frac{dv(x)}{dx} > 0 \quad \text{for } 0 < x < x_1$$

Under the assumptions [7], for any $p_- > 0$, where $E = p_-^2/2 < v(x_1)$, eqn [1] has a unique solution $x \in C^2(\mathbb{R},]-\infty, x_1])$ such that

$$x(t) = p_- t \quad \text{for } t \leq 0 \qquad [8]$$

in addition,

$$x(t) = -p_- t + b(p_-) \quad \text{as } t \to +\infty \qquad [9]$$

Let

$$T(E) = \frac{b(\sqrt{2E})}{\sqrt{2E}}, \quad 0 < E < v(x_1), \ \sqrt{2E} > 0 \qquad [10]$$

($T(E)$ is the time during which a particle starting at $x = 0$ with the impulse $p_- = \sqrt{2E}$ returns to $x = 0$).

Let $x(v)$, $v \in [0, v(x_1)]$, be the inverse function to $v(x)$, $x \in [0, x_1]$. Then (under the assumptions [7]),

$$T(E) = \sqrt{2} \int_0^E (E - v)^{-1/2} \frac{dx(v)}{dv} dv$$
$$0 < E < v(x_1) \qquad [11]$$

$$x(v) = \frac{1}{\sqrt{2}\pi} \int_0^v (v - E)^{-1/2} T(E) dE$$
$$0 < v < v(x_1) \qquad [12]$$

Actually, the formulas [11], [12] relating the travel time T and the potential v are the results from Abel (1826) (see also Keller (1976) for a discussion of this result). Formula [11] is a result on direct scattering, whereas [12] is a result on inverse scattering. In addition, if $T(E), 0 < E < v(x_1)$, is given, then [11] is the Abel integral equation for $x(v), 0 < v < v(x_1)$, and [12] solves this equation.

Concerning further results on inverse scattering for the one-dimensional Newton equation, see Keller (1976) and Astaburuaga *et al.* (1991). Note that for the one-dimensional case the scattering data a, b do not in general determine v uniquely.

The Abel integral equation and the Abel formula solving this equation were used also, in particular, by Firsov (1953) and Keller *et al.* (1956), where inverse scattering was considered for the three-dimensional Newton equation at fixed energy for the case of spherically symmetric monotonous decreasing potential in $|x|$.

Note also that the Abel method for solving the integral equation [11] was used by Radon (1917) for finding the inversion formula for the Radon transformation. In the next section, we reduce the inverse-scattering problem for the Newton equation [1] in dimension $d \geq 2$, under the assumptions [2], to the inversion problem for the X-ray transformation (i.e., the Radon transformation along straight lines).

Inverse Scattering for the Multidimensional Newton Equation

Consider

$$T\mathbb{S}^{d-1} = \{(\theta, x) \in \mathbb{S}^{d-1} \times \mathbb{R}^d \mid \theta x = 0\} \quad [13]$$

Consider the X-ray transformation P defined by the formula

$$Pf(\theta, x) = \int_{\mathbb{R}} f(t\theta + x)\mathrm{d}t, \quad (\theta, x) \in T\mathbb{S}^{d-1} \quad [14]$$

where

$$f \in C(\mathbb{R}^d, \mathbb{R}^m)$$
$$f(x) = O(|x|^{-\beta}) \quad \text{as } |x| \to \infty \text{ for some } \beta > 1 \quad [15]$$

Consider the functions $a_{\mathrm{sc}}, b_{\mathrm{sc}}$ of [6]

Theorem 1 (Novikov 1999). *For the Newton equation* [1], *under the assumptions* [2], *the following formulas hold*:

$$PF(\theta, x) = \lim_{s \to +\infty} s a_{\mathrm{sc}}(s\theta, x), \quad (\theta, x) \in T\mathbb{S}^{d-1} \quad [16]$$

$$Pv(\theta, x) = \lim_{s \to +\infty} s^2 \theta b_{\mathrm{sc}}(s\theta, x), \quad (\theta, x) \in T\mathbb{S}^{d-1} \quad [17]$$

in addition,

$$|PF(\theta, x) - s a_{\mathrm{sc}}(s\theta, x)| \le \frac{d^3 c^2 2^{2\alpha+4}}{\alpha(\alpha-1)(1+|x|/\sqrt{2})^{2\alpha-1}} \frac{s^3}{(s/\sqrt{2}-1)^4} \quad [18]$$

$$|Pv(\theta, x) - s^2 \theta b_{\mathrm{sc}}(s\theta, x)| \le \frac{d^3 c^2 2^{2\alpha+4}}{\alpha(\alpha-1)^2(1+|x|/\sqrt{2})^{2\alpha-2}} \frac{s^4}{(s/\sqrt{2}-1)^5} \quad [19]$$

for $(\theta, x) \in T\mathbb{S}^{d-1}, s \ge z(d, c, \alpha, |x|)$, *where* θb_{sc} *is the scalar product of* θ *and* b_{sc}, z *is the root of the equation*

$$\frac{d^2 c 2^{\alpha+2}}{(\alpha-1)(1+|x|/\sqrt{2})^{\alpha-1}} \frac{z^2}{(z/\sqrt{2}-1)^3} = 1$$
$$z \in]\sqrt{2}, +\infty[\quad [20]$$

$c = \max(c_1, c_2)$ (*and* α, c_1, c_2 *are the constants of* [2]).

Theorem 1 gives a method for finding PF and Pv from a_{sc} and b_{sc} at high energies. It has been proved in Novikov (1999) by means of analysis of the following nonlinear integral equation for the function y_- of [3]:

$$y_-(t) = A_{p_-, x_-}(y_-)(t)$$

where

$$A_{p_-, x_-}(u)(t) = \int_{-\infty}^{t} \int_{-\infty}^{\tau} F(p_- s + x_- + u(s))\mathrm{d}s\,\mathrm{d}\tau$$
$$p_- \neq 0$$

In dimension $d \ge 2$, Theorem 1 and methods for the reconstruction of f from Pf (Gelfand *et al.* 1980, Natterer 1986, Novikov 1999) give a method for the reconstruction of F and v from the scattering data a, b at high energies. Note that for $d = 1$ Theorem 1 is valid but f cannot be uniquely reconstructed from Pf.

Theorem 1 is an analog of the Born formula for the Schrödinger equation at high energies (see, e.g., Faddeev (1956), Enss and Weber (1995), and Novikov (1998) as regards this Born formula and its variations). On the other hand, Theorem 1 was preceded by a result of Gerver and Nadirashvili (1983) on the high-energy asymptotics for the travel time between boundary points for the Newton equation in a bounded strictly convex domain with smooth boundary. There is a considerable similarity between this result and Theorem 1.

We continue our review on inverse scattering for the multidimensional Newton equation, and make the following well-known observation.

Observation 1 *Suppose that* $v(x) > E > 0$ *for* $x \in \mathcal{U}$, *where* $\mathcal{U}$ *is a compact subset of* $\mathbb{R}^d$. *Then the scattering data* a, b *for energies smaller than or equal to* E *contain no information about* $v(x)$ *for* $x \in \mathcal{U}$.

In addition to Theorem 1 and Observation 1, one has the following conjecture.

Conjecture 1 (Novikov 1999). *Suppose that* v *satisfies* [2], $d \ge 2$, *and the energy* E *is sufficiently large*, $E > E(v)$. *Then the scattering data* a, b *at fixed energy* E *uniquely determine* v.

Gerver and Nadirashvili (1983) proved a result similar to Conjecture 1 for the case of the Newton equation in a bounded strictly convex domain G with smooth boundary. Their proof of this result contains no reconstruction method but does contain a stability estimate. It is based on the Maupertuis principle and the results of Muhometov and Romanov (1978), Beylkin (1979), and Bernstein and Gerver (1980). For the case $v \in C^2(\mathbb{R}^d, \mathbb{R})$, $\operatorname{supp} v \subset G$ (where G has the properties mentioned above), in Novikov (1999) a connection between the boundary-value data of Gerver and Nadirashvili (1983) and the scattering data a, b is given and it is shown that for $d \ge 2$ the scattering data a, b and the domain G uniquely determine v at fixed sufficiently large energy $E > E(v, G)$.

For more information concerning results mentioned above, see Novikov (1999) and Gerver and Nadirashvili (1983). One can see from the review of this section that very few results on inverse scattering for the multidimensional Newton equation are given in the literature, at present. It should

be remarked that the inverse-scattering theory in multidimensions is much more developed for the Schrödinger equation than for the Newton equation.

Inverse Scattering for the Schrödinger Equation in Multidimensions

The inverse-scattering theory for the multidimensional Schrödinger equation has been developed by many authors (see, e.g., surveys given in Grinevich (2000) and Novikov (2001)).

Quantum-mechanical analogs of Theorem 1 appear, for example, in Faddeev (1956), Enss and Weder (1995), Novikov (1998) (see also references therein). Similarly, the quantum-mechanical analogs of Conjecture 1 have been proved, for example, in Novikov (1992, 1994) and Grinevich and Novikov (1995) (see also references therein). On the other hand, as a rule, classical-mechanical analogs of results of the works on inverse Schrödinger scattering in multidimensions are unknown. This leads to many open problems. For the one-dimensional case some results on finding classical limits of results on inverse Schrödinger scattering are given in Lax and Levermore (1983) and Bogdanov (1985). Note that inverse scattering for the two-dimensional Schrödinger equation at fixed energy (see Novikov (1992), Grinevich and Novikov (1995), and Grinevich (2000) and references therein) has considerable similarity with inverse scattering for the one-dimensional Schrödinger equation. Therefore, an interesting open problem consists in extending the aforementioned study of Lax and Levermore (1983) and Bogdanov (1985) to the case of inverse scattering for the two-dimensional Schrödinger equation at fixed energy. Perhaps, in this way one can find proper two-dimensional analogs of the Abel formulas [11] and [12].

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Inverse Problems in Wave Propagation *see* Boundary Control Method and Inverse Problems of Wave Propagation

Inviscid Flows

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Introduction

The equations governing the motion of an ideal (inviscid) fluid were derived by Euler in 1755. They were, together with the equation of vibrating strings, the first partial differential equations introduced in the field of mathematical physics. While several partial differential equations, coming from the modeling of physical phenomena, have had a satisfactory mathematical solution, it is piquant to note that the old Euler equations remain essentially unsolved. Together with the Navier–Stokes equations of viscous fluids, the Euler equations play a central role in the modern analysis of partial differential equations.

The mathematical difficulties encountered in the study of Euler equations seem to be deeply linked with the understanding of turbulence, which remains one of the great open problems in the field of macroscopic physics.

The relevance of Euler equations as a model of fluid flow is rather subtle, and the discussion is far from closed. On the one hand, Euler equations have disturbing aspects, which, in their most visible form, yield paradoxes. On the other hand, the systematic recourse to some viscosity seems to put a serious obstacle to a proper understanding of turbulence. In this article we will try to give some insight into this issue.

To be rigorous, every fluid has some compressibility, that is to say the density varies with the pressure. Compressibility gives rise to pressure waves, which propagate in the fluid with some finite speed. When the velocity of the fluid particles is slow relative to the speed of the pressure waves, it is legitimate to make the approximation that the flow is incompressible; it is the case for meteorological flows, for example. Then, there are no more pressure waves; nevertheless the motion can be very unstable and intricate (turbulent). Although very often in physical flows these two features coexist, following the tradition, we clearly separate the compressible and incompressible cases.

The Equations of the Perfect Fluid

Until now a rigorous derivation of the fluid equations from a system of interacting particles governed by Newton's laws is not known. Thus, the mathematical models of fluid motion result from heuristic considerations.

Let us specify some notations.

The fluid motion is supposed to take place in some domain (not necessarily bounded) Ω of the physical space $\Re^3$.

We shall use the so-called Eulerian description of the fluid motion: $\rho(t,x)$ denotes the local density of the fluid at time t and position x, and $u(t,x)$ the velocity of the fluid particle located at x at time t.

The first equation (conservation equation) expresses the conservation of mass:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0 \qquad [1]$$

The second equation (momentum equation) expresses Newton's law (in the absence of internal friction):

$$\rho\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u\right) = -\nabla p \qquad [2]$$

where the scalar function p(t, x) is the pressure inside the fluid, and

$$(u \cdot \nabla)u = \sum_i u_i \partial_i u$$

With [1] and [2], we have five scalar unknown functions (ρ, u_i, p) and only four equations. To get a

closed set of equations, we need to add a supplementary relationship:

$$\operatorname{div}(\boldsymbol{u}) = 0, \quad \text{for the incompressible flows} \quad [3]$$

In the case of compressible flows, eqns [1] and [2] must be completed by a thermodynamical description of the fluid, which yields a relationship between ρ, p, the internal energy, the specific entropy, etc. We will only consider here the simple case of an isentropic gas which is modeled by the relationship

$$p = p(\rho) \quad [4]$$

with $p(\rho) = c\rho^{\gamma}$ for a perfect gas $(c > 0, \gamma > 1)$.

Condition at the Boundary $\partial\Omega$ of the Domain

In the case of a perfect fluid, we simply have to write that the velocities of the fluid particles at the boundary are tangent to the boundary, that is,

$$\boldsymbol{u} \cdot \boldsymbol{n} = 0 \quad \text{on } \partial\Omega \quad [5]$$

where $\boldsymbol{n}$ denotes the unit normal vector to the boundary (pointing outward).

The Incompressible Perfect Fluid: Main Properties of Smooth Flows

We shall suppose $\rho = 1$. Equations [1]–[3] and [5] then yield the classical Euler system:

$$\begin{aligned} &\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p \quad \text{on } \Omega \\ &\operatorname{div} \boldsymbol{u} = 0, \quad \boldsymbol{u} \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega \end{aligned} \quad [6]$$

The Constants of the Motion

Let us examine the constants of the motion of the dynamical system defined by [6], that is, the functionals which are conserved by the motion of the fluid.

First we have the classical constants of motion associated with the natural symmetries by Noether's theorem.

The time translational invariance of the system implies that the kinetic energy is conserved:

$$E_c = \frac{1}{2}\int_{\Omega} u^2 \, \mathrm{d}x$$

In the case $\Omega = \Re^3$, the homogeneity of space implies the conservation of the impulsion:

$$\int_{\Omega} \boldsymbol{u} \, \mathrm{d}x$$

The space isotropy, on the other hand, yields the conservation of the angular momentum:

$$\int_{\Omega} \boldsymbol{x} \wedge \boldsymbol{u} \, \mathrm{d}x$$

There is a more hidden constant of the motion, called helicity, which was discovered in 1961 by J J Moreau (1961) (see, e.g., Serre (1979)).

Let us define the vorticity of the flow:

$$\omega = \operatorname{curl} \boldsymbol{u}$$

then the helicity is

$$\int_{\Omega} \omega \cdot \boldsymbol{u} \, \mathrm{d}x$$

Of course, here, we suppose $\boldsymbol{u}$ to be vanishing at infinity in such a manner that the above integrals make sense.

One may wonder about the existence of other constants of the motion of the form (first-order functionals):

$$\int F(\boldsymbol{x}, \boldsymbol{u}(\boldsymbol{x}), \nabla \boldsymbol{u}(\boldsymbol{x}))\mathrm{d}x$$

The answer, due to Serre (1979), is that any functional of the above form which is conserved by the flow is a linear function of the energy, the impulsion, the angular momentum, the helicity plus a trivial term (i.e., taking the same value for any field $\boldsymbol{u}$ such that $\operatorname{div} \boldsymbol{u} = 0$).

Beltrami Equation and Kelvin's Theorem

Another important issue is to know how the vorticity field evolves in a regular flow. If we apply the operator curl to the equation [6] in order to eliminate the pressure term, we get:

$$\frac{\partial \omega}{\partial t} + (\boldsymbol{u} \cdot \nabla)\omega - (\omega \cdot \nabla)\boldsymbol{u} = 0 \quad [7]$$

which is the Beltrami equation.

To exploit the Beltrami equation, we need the Lagrangian flow $\varphi(t, \boldsymbol{x})$, associated with the field $\boldsymbol{u}$, which is defined by the differential equation:

$$\frac{\partial \varphi}{\partial t}(t, \boldsymbol{x}) = \boldsymbol{u}(t, \varphi(t, \boldsymbol{x})), \quad \varphi(0, \boldsymbol{x}) = \boldsymbol{x}$$

Then we can state the following proposition.

Proposition *During the smooth motion of an incompressible perfect fluid, we have:*

$$\omega(t, \varphi(t, \boldsymbol{x})) = D\varphi(t, \boldsymbol{x})[\omega(0, \boldsymbol{x})], \quad \text{for all } t, \boldsymbol{x}$$

where $D\varphi(t, \boldsymbol{x})$ denotes the derivative at the point $\boldsymbol{x}$ (t fixed) of the mapping $\boldsymbol{x} \to \varphi(t, \boldsymbol{x})$.

The first consequence of this result is to point out the class of irrotational flows, for which

$\omega(t, x) = 0$. Indeed, if the vorticity vanishes initially, it follows from the proposition that it will vanish for ever.

Another consequence is the behavior of vortex lines. By definition, a vortex line is any integral curve of the vorticity field. More precisely, a vorticity line at time t, $C(s)$ is defined by the differential equation

$$\frac{dC}{ds}(s) = \omega(t, C(s))$$

Now we can check that vortex lines are merely transported by the flow: if $C(s)$ is a vortex line at time $t = 0, \varphi(t, C(s))$ is a vortex line at time t.

We end this section with the famous Kelvin's circulation theorem (1869) (see, e.g., Marchioro and Pulvirenti (1994)).

Theorem *Let L be a closed (oriented) contour drawn inside the fluid. We suppose that L is transported by the flow; $\varphi_t(L)$ denotes the contour at time t. Then the circulation of the velocity field $u(t, x)$ along $\varphi_t(L)$ is independent of t.*

Stationary Solutions: D'Alembert's Paradox

Let us focus now on the flow around a bounded body $\overline{\Omega}$, whose complement $\overline{\Omega}^c$ will be supposed to be simply connected.

A stationary solution $u(x), p(x)$ satisfies:

$$(u \cdot \nabla)u = -\nabla p$$
$$\operatorname{div} u = 0, \quad u \cdot n = 0 \quad \text{on } \partial\Omega$$

But since $(u \cdot \nabla)u = \nabla(\frac{1}{2}u^2) + (\operatorname{curl} u) \wedge u$, any stationary field $u(x)$ satisfying curl $u = 0$, div $u = 0$, $u \cdot n = 0$ on $\partial\Omega$, defines a stationary solution with associated pressure $p = -\frac{1}{2}u^2$.

We also need to specify a condition at infinity for the field u. We impose that the velocity is equal (at infinity) to some constant value U. Since $\overline{\Omega}^c$ is simply connected, the condition curl $u = 0$ implies that the flow is potential, that is, there is a scalar function $F(x)$ such that $u = U + \nabla F$.

Thus, the determination of an irrotational flow around an obstacle amounts to solving the following exterior Neuman problem.

Find F satisfying:

$$\Delta F = 0 \quad \text{in } \overline{\Omega}^c$$
$$\frac{\partial F}{\partial n} = -U \cdot n \quad \text{on } \partial\Omega$$
$$\nabla F = 0 \quad \text{at infinity}$$

This problem is well known and has a unique solution, which satisfies, at infinity:

$$F(x) = O(1/|x|^2) \qquad \nabla F(x) = O(1/|x|^3)$$

Then a classical calculation (integration by parts) gives the resulting force exerted by the flow on the body:

$$R = -\int_{\partial\Omega} pn \, d\sigma = \int_{\partial\Omega} \frac{1}{2} u^2 n \, d\sigma = 0$$

This property of inviscid potential flows was first noticed by Jean Le Rond d'Alembert (1717–1783). Furthermore, d'Alembert performed a series of experiments to measure the drag on a sphere in a flowing fluid and he expected that the force would go to zero as the viscosity of the fluid approached zero. But this was not the case: the drag seemed to converge toward a nonzero value. Hence, this property was called d'Alembert's paradox.

Of course, d'Alembert's paradox tells us that something is going wrong: this model of flow around a body is not physically relevant. But it is not obvious to identify precisely what is going wrong.

Physics tells us that in a flow around a flying airplane, the viscous term (as measured by an dimensionless number called Reynolds number) is very small. The main effect of the viscosity is then to alter the limit condition at the boundary of the body. The relevant boundary condition is no longer $u \cdot n = 0$, but the purely viscous condition $u = 0$, or more realistically a condition of friction type (turbulent boundary condition).

A common approach is to disqualify the perfect-fluid model in arguing that this modification of the boundary condition has important consequences on the flow near the body (giving rise to a turbulent boundary layer, for example).

It seems to us that such a disqualification of the perfect-fluid model discards prematurely interesting issues. Indeed, we must notice first that the stationary solution on which d'Alembert's reasoning is based is highly unstable and not acceptable physically. Thus, a realistic solution would necessarily be either nonstationary or with some vorticity. On this basis, we can imagine other scenarios to explain the existence of a resulting force exerted on the body. For example, we may imagine a stationary solution with a discontinuous velocity field (i.e., with a vortex sheet). The process conducive to such a stationary solution is called Prandtl's scenario (Batchelor 1967). The mathematical proof that Prandtl's scenario does exist is a difficult (open) issue, which seems closely related to the (probable) nonuniqueness of weak solutions of the Cauchy problem.

The Cauchy Problem for the Incompressible Perfect Fluid

The Case $\Omega \subset \Re^3$

In the Cauchy problem, given an initial velocity field $\boldsymbol{u}_0(\boldsymbol{x})$, we want to determine the corresponding solution $\boldsymbol{u}(t,\boldsymbol{x})$ of [6] at each time t.

The first significant result on the Cauchy problem for three-dimensional Euler equations was given by Kato (1975).

Theorem *For $\boldsymbol{u}_0$ in the Sobolev space $H^s(\Re^3)$, for $s > 5/2$, there is $T > 0$ and a unique classical solution (of the Cauchy problem) $\boldsymbol{u}(t,\boldsymbol{x})$ on $[0,T] \times \Re^3$. $\boldsymbol{u}$ depends continuously on t in the space H^s.*

By a classical solution we mean that the field $\boldsymbol{u}(t,\boldsymbol{x})$ is derivable in terms of the variables t, $\boldsymbol{x}$ and satisfies the equations in the usual sense.

Here $H^S(\Re^3)$ denotes the Sobolev space of the fields $\boldsymbol{u}$, which are square integrable and with spatial derivatives of order s (in the case where s is an integer) also square integrable.

Remark These results have been generalized to some extent during the last few decades, but the following issues are still open:

1. Do singularities occur at a finite time for such regular solutions?
2. For a less regular initial datum, do weak solutions exist (in the sense of distributions)?

The Case $\Omega \subset \Re^2$

This case is better understood, the first mathematical results trace back to Lichtenstein (1925) and Wolibner (1933); they take a plain form with the famous theorem of Youdovitch 1963 (see, e.g., Chemin (1995)).

In two dimensions, the vorticity $\omega = \operatorname{curl} \boldsymbol{u}$ identifies with a scalar function, and the Beltrami equation becomes

$$\frac{\partial \omega}{\partial t} + \operatorname{div}(\omega \boldsymbol{u}) = 0 \qquad [8a]$$

$$\operatorname{curl} \boldsymbol{u} = \omega \qquad [8b]$$

$$\operatorname{div} \boldsymbol{u} = 0, \quad \boldsymbol{u} \cdot \boldsymbol{n} = 0 \quad \text{on } \partial\Omega \qquad [8c]$$

This formulation, which appears as a transport equation [8a] for ω, coupled with the elliptic system [8b]–[8c], which determines $\boldsymbol{u}$ from ω, is particularly convenient.

The constants of motion associated with the usual symmetries, of course, persist; notice, however, that the helicity degenerates since, in two dimensions, $\omega \cdot \boldsymbol{u} = 0$. But now from [8a] we see that ω is merely convected by the incompressible velocity field $\boldsymbol{u}$. We deduce that, for any continuous function f, the functional

$$\int_\Omega f(\omega(t,\boldsymbol{x}))\mathrm{d}\boldsymbol{x}$$

is a constant of motion.

Thus, a specific feature of the two-dimensional case is to introduce an infinite set of constants of motion. By a skilful exploitation of this fact, Youdovitch succeeded in proving the following result.

Theorem *For a given ω_0 in the space $L^\infty(\Omega)$, there is a unique weak solution $\omega(t,\boldsymbol{x})$ of [8], such that $\omega(t,\boldsymbol{x})$ is in $L^\infty(\Omega)$ for all t, and ω depends continuously on t in the space $L^p, 1 \le p < \infty$.*

L^p denotes, in a standard way, the Lebesgue space of the functions f such that $|f|^p$ is integrable over Ω and $L^\infty(\Omega)$, the space of measurable bounded functions on Ω.

Thus, if we limit ourselves to initial data with bounded scalar vorticity, the Cauchy problem for the two-dimensional incompressible perfect fluid is satisfactorily solved. The situation is much more intricate if we consider a less regular initial datum (e.g., if ω_0 is a measure supported by a curve (vortex sheet)).

Arnol'd's Work on Two-Dimensional Inviscid Flows

Youdovitch's theorem implies that the incompressible Euler equations, with ω_0 in $L^\infty(\Omega)$, is a satisfactory model of two-dimensional flows – an important issue to study further the properties of this model.

A famous result due to Arnol'd (see Arnol'd and Khesin (1998) and Marchioro and Pulvirenti (1994)) deals with the nonlinear stability of the stationary solutions.

Let us determine the smooth stationary solutions of the two-dimensional Euler equations in a bounded domain Ω of the plane. We have to solve:

$$(\boldsymbol{u} \cdot \nabla)\omega = 0 \qquad [9a]$$

$$\operatorname{curl} \boldsymbol{u} = \omega \qquad [9b]$$

$$\operatorname{div} \boldsymbol{u} = 0, \quad \boldsymbol{u} \cdot \boldsymbol{n} = 0 \quad \text{on } \partial\Omega \qquad [9c]$$

Since we have div $\boldsymbol{u} = 0$, we may introduce the stream function of $\boldsymbol{u}$, ψ, which is given by the Dirichlet's problem:

$$-\Delta\psi = \omega, \quad \psi = 0 \text{ on } \partial\Omega$$

so that $\boldsymbol{u} = \operatorname{curl} \psi$.

The system [9] becomes:

$$\nabla\psi \wedge \nabla\omega = 0, \quad -\Delta\psi = \omega, \quad \psi = 0 \text{ on } \partial\Omega$$

Let us focus on solutions which are characterized by a relationship $\omega = f(\psi)$, where f is a smooth function. Such solutions are given by the resolution of the following nonlinear elliptic problem:

$$-\Delta\psi = f(\psi), \quad \psi = 0 \text{ on } \partial\Omega \qquad [10]$$

This problem has always at least a solution, for example, if f is a bounded function of ψ.

Let ψ^* be a solution of [10], and $\omega^* = f(\psi^*)$ the corresponding vorticity function. We shall say that the stationary solution ω^* is stable in the L^2-norm if:

For all $\varepsilon > 0$, there is a $\delta > 0$, such that for all initial datum ω_0 in $L^\infty(\Omega)$ satisfying

$$\int_\Omega (\omega^* - \omega_0)^2 \mathrm{d}x \le \delta, \text{ we have :}$$

$$\int_\Omega (\omega^* - \omega(t))^2 \, \mathrm{d}x \le \varepsilon, \text{for all } t$$

where $\omega(t)$ denotes the solution of the Cauchy problem associated with the initial datum ω_0 by Youdovitch's theorem.

Now we can state the following result.

Theorem (Arnol'd) *Let ω be a stationary solution given by* [10]. *We assume that one of the following assumptions holds*:

(C1) *There are positive constants c_1, c_2, such that*

$$c_1 \le f' \le c_2$$

(C2) *There are positive constants c_1, c_2, with $c_2 < \lambda_1$ (first eigenvalue of the Dirichlet problem on the domain Ω) such that*:

$$c_1 \le -f' \le c_2$$

Then ω is stable in the L_2-norm.

Remarks

(i) This result was the first nonlinear stability result for stationary flows.
(ii) The proof makes use of the conservation of the functionals of the vorticity field.

Another significant contribution of Arnol'd to hydrodynamics was to reveal the geometrical aspect of the instability of the perfect-fluid motion. We give a brief insight into this issue.

Let us come back to the Lagrangian description of motion. We want to determine the function $\varphi(t, x)$. Each mapping $\varphi_t(x) = \varphi(t, x)$ is, for t fixed, a diffeomorphism of $\bar{\Omega}$ preserving the Lebesgue measure and the orientation (equivalently stated, it is an element of $\mathrm{SDiff}(\bar{\Omega})$).

In other words, a fluid motion is a curve $t \to \varphi_t$ drawn on the "manifold" $M = \mathrm{SDiff}(\bar{\Omega})$ (the configuration space of the system).

At time t, the relationship

$$\frac{\partial\varphi}{\partial t}(t, x) = u(t, \varphi(t, x))$$

states that the velocity field $u(t, \varphi_t(x))$ belongs to the space tangent to M at φ_t. The tangent space at φ to M is the space of vector fields $v(\varphi(x))$, where $v(x)$ is an incompressible vector field on $\bar{\Omega}$ satisfying $v \cdot n = 0$ on $\partial\Omega$. This space is naturally endowed with a norm given by the kinetic energy

$$\frac{1}{2}\int_\Omega v(x)^2 \mathrm{d}x$$

and thus M is endowed with a Riemannian structure.

It is easy to check that the perfect-fluid motions correspond to the curves φ_t drawn on M which are the critical points of the action integral:

$$\frac{1}{2}\int_{t_1}^{t_2} \mathrm{d}t \int_\Omega \left|\frac{\partial\varphi}{\partial t}(t, x)\right|^2 \mathrm{d}x, \quad \text{for all } t_1 < t_2$$

$$\text{(with the constraints } \varphi(t_1, .) = \varphi_1, \varphi(t_2, .) = \varphi_2)$$

That is to say, the perfect-fluid motions are the geodesics of the Riemannian manifold M.

The main interest of this geometric framework is to bring back, at least formally, the perfect-fluid motions to well-known objects. Indeed, we know that the Riemannian curvature of a manifold has a profound impact on the behavior of geodesics on it. If the Riemannian curvature is positive, then nearby geodesics oscillate about one another, and if the curvature is negative, geodesics rapidly diverge from one another. More precisely, the stability of geodesics is expressed in terms of the curvature by means of Jacobi's equation [1]. If φ_t is a geodesic curve starting from φ_0, with velocity field $v(t)$ (whose norm is supposed equal to 1), if the sectional curvature of the manifold in all the 2-planes containing $v(t)$ is less than $-c(<0)$, a perturbation of the initial datum will increase at least as $\exp(ct)$:

$$d(\varphi_t, \tilde{\varphi}_t) \ge d(\varphi_0, \tilde{\varphi}_0)\exp(ct)$$

where $\tilde{\varphi}_0$ denotes the perturbed initial datum and d the geodesic distance on the manifold. Moreover, if the curvature at every point and for all the sections is less than $-c$, and if M is compact, then the geodesic flow, that is, the one-parameter group of transformations $(\varphi_0, v(0)) \to (\varphi_t, v(t))$, is mixing (in the usual meaning of ergodic theory). Arnol'd succeeded in calculating the sectional curvature for flows on the two-dimensional torus; he showed that the

curvature is negative for "most" of the sections. This gives an enlightening geometrical picture of the instability of Lagrangian flows.

It was tempting to connect the above considerations on the instability of two-dimensional flows with the problem of weather forecast. In 1963 EN Lorenz stated that a two-week forecast would be a theoretical bound for predicting the atmospheric motion. Lorenz's assertion was based on numerical simulations. He took as model for the large-scale atmospheric motion the two-dimensional Euler equations on the torus, which he truncated to a small number of Fourier modes (about 20). This model is highly unstable and displays exponential sensitivity with respect to the initial datum. However, the parallel between the behavior of this system and the instability of the Lagrangian flow is misleading. On the one hand, if we again do the Lorenz computations on Euler equations, taking into account a large number of Fourier modes, we note a striking phenomenon: the flow has a tendency to self-organize into large vortices, called coherent structures, and simultaneously the exponential sensitivity, as measured in terms of the energy norm of the velocity field, disappears. On the other hand, the problem of predicting the Lagrangian flow is very different, the Lagrangian flow can be exponentially unstable, while the corresponding velocity field quietly converges, in the energy norm, towards some equilibrium. We must keep in mind that the meteorologist aims to predict the values of the velocity field at some future time and not the trajectories of the fluid particles. In fact, it appears that Lorenz has ignored phenomena of a statistical nature which occur when a large number of degrees of freedom are considered; thus, his theoretical bound for the prediction of the atmospheric motion has no definite basis. More detailed reflections on this issue can be found in Robert and Rosier (2001).

The Cauchy Problem for the Euler Equations for Compressible Inviscid Fluids

As remarked in the introduction, compressible flows yield pressure waves. The equations of motion being nonlinear, these waves interact in an intricate manner giving rise to shocks. This is the main feature of compressible fluid flows. Compressible flows are situated in the more general domain of nonlinear hyperbolic systems, which were intensively studied during the last decades. We only give here an example of the kind of result which can be obtained.

The following theorem, which states that for a set of regular initial data, shocks do not occur till some finite time, is a consequence of a more general result on hyperbolic systems due to Majda (1984).

We consider $\Omega = \Re^3$ and the system [1], [2], [4].

Theorem *Assume* $p_0, \boldsymbol{u}_0 \in H^S \cap L^\infty(\Re^3)$, *with* $s > 5/2$ *and* $p_0(\boldsymbol{x}) > 0$. *Then there is a finite time* $T > 0$, *depending on the* H^s *and* L^∞ *norms of the initial data, such that the Cauchy problem for* [1], [2], [4] *has a unique bounded smooth solution* p, $\boldsymbol{u} \in C^1([0,T] \times \Re^3)$, *with* $p(t,\boldsymbol{x}) > 0$ *for all* $t, \boldsymbol{x}$.

Inviscid Flows and Turbulence

Loosely speaking, turbulence is the intricate motion of a slightly viscous flow. Going back to the first half of the last century, there are two main approaches to turbulence. The first is due to Leray. The dissipation of energy is a characteristic feature of three-dimensional turbulence, and Leray thought that, even if very small, the viscosity of the fluid plays an important role, so that to understand turbulence the first step is to study the Navier–Stokes equations. A radically different approach is due to Onsager. Onsager (1949) started with the fundamental remark that the 4/5 law of turbulence, which relates the dissipation of energy to the increments of the velocity field, does not involve viscosity. Furthermore, he observed that the proof of the conservation of energy for the solutions of Euler equations uses an integration by parts which supposes some regularity of the velocity field. He then imagined that an inviscid dissipation mechanism, due to a lack of regularity of the solutions, was at work in Euler equations. In modern terminology, he suggested to model turbulent flows by nonregular (weak) solutions satisfying the Euler equations in the sense of distributions. He also conjectured that if a solution satisfies a Hölder regularity condition of order $>1/3$, then the energy would be conserved.

Onsager's views were revolutionary and forgotten for a long time. Recent works, such as the proof of Onsager's conjecture, the construction of weak solutions with energy dissipation, and the discovery of the explicit local form of the energy dissipation for weak solutions, show a renewed interest in these views (see, e.g., Constantin and Titi (1994), Eyink (1994), Robert (2003), and Shnirelman (2003)).

See also: Compressible flows: Mathematical Theory; Dissipative Dynamical Systems of Infinite Dimension; Hyperbolic Dynamical Systems; Incompressible Euler Equations: Mathematical Theory; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Chaos and Attractors; Turbulence Theories.

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Ising Model *see* Two-Dimensional Ising Model

Isochronous Systems

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Introduction

This paper reviews recent developments, following closely (sometimes *verbatim*) the review paper Calogero F (2004c) (see the Bibliography below); for more traditional investigations of *isochronous* systems see other entries of this Encyclopedia (and for the mathematical investigation of isochronous centers in the plane, related to the 16th Hilbert problem, see for instance the survey paper referred to at the end of this entry).

The *isochronous* systems treated herein are characterized by the property to possess an *open* domain having full dimensionality in their phase space such that *all* the motions evolving from a set of initial data in it are *completely periodic* with the same fixed period. The natural measure of this *open* domain might, or it might not, be *infinite* when the measure of the entire phase space is itself *infinite*: for instance, if the entire phase space is the two-dimensional Euclidian plane, such a domain might be the exterior, or the interior, of a circle of finite radius.

It is justified to call such systems *superintegrable*, or perhaps *partially superintegrable* inasmuch as the property of *isochronicity* of all their motions holds only in a subregion of the entire phase space. This terminology is justified by the observation that, roughly speaking, all confined motions of a *superintegrable* system – in which all but one of the degrees of freedom are constrained by the existence of the *maximal* possible number of constants of motion – are *completely periodic*, although not necessarily all with a fixed period – entailing that *isochronicity* entails *superintegrability*, while the converse is not the case (see the entry *Integrable systems* in this Encyclopedia).

A simple trick – amounting essentially to a change of independent, and possible as well of dependent, variables, allows to deform a largely arbitrary dynamical system so that the deformed system obtained from it be *isochronous*. This "trick", which is now explained, entails therefore that *isochronous systems are not rare*. Below we provide several examples; others can be found in the further reading suggested at the end of this entry, and/or can be manufactured *ad libitum* using the trick.

The Trick

We now show that, given a largely arbitrary dynamical system, it is possible to introduce a deformed version of it featuring a *real* constant ω, that has the following properties: for $\omega = 0$, it coincides with the original, undeformed system; for $\omega > 0$, it possesses an *open* region having full dimensionality in its phase space such that *all* solutions evolving from an initial datum in it are *completely periodic* with a period $\tilde{T}$ which is a finite integer multiple, or perhaps a simple fraction, of the basic period

$$T = \frac{2\pi}{\omega} \qquad [1]$$

Let us indeed, consider a quite general dynamical system which we write as follows:

$$\zeta' = F(\zeta; \tau) \qquad [2]$$

Here $\zeta \equiv \zeta(\tau)$ is the dependent variable, which might be a scalar, a vector, a tensor, a matrix, you name it. The independent variable is τ, and the main limitation on the dynamical system [2] is that it be permissible to treat this variable as *complex*; this requires that the derivative with respect to this *complex* variable τ that appears in the left-hand side of the evolution equation [2] make sense, namely that this dynamical system be *analytic*, entailing that the dependent variable ζ be an *analytic* function of the complex variable τ (but this does not require $\zeta(\tau)$ to be a holomorphic nor a meromorphic function of $\tau; \zeta(\tau)$ might feature all sorts of singularities, including branch points, in the complex τ-plane, indeed this will generally happen since we generally assume the evolution equation (??) to be *nonlinear*). The quantity F in the right-hand side of [2] – which has of course the same scalar, vector, matrix... character as ζ – might depend (arbitrarily but analytically) on ζ as well as on τ. (Let us also emphasize that this approach is as well applicable to more general dynamical systems that also feature other, "spacelike", independent variables, for instance are a system of PDEs rather than ODEs; the interested reader is referred to the literature cited below).

In spite of the generality of this dynamical system, [2], there generally holds a result ("Theorem of existence, uniqueness and analyticity") that characterizes the solution $\zeta(\tau)$ of its initial-value problem determined by the assignment

$$\zeta(0) = \zeta_0$$

Here, for notational simplicity, we assign the initial datum ζ_0 at $\tau = 0$; and we assume of course that the right-hand side of [2] is not singular for $\tau = 0$ and $\zeta = \zeta_0$. The relevant result guarantees, not only for the initial datum ζ_0, but for a (sufficiently small but open) set of initial data in its neighborhood, the existence of a circular disk in the complex τ-plane, centered at $\tau = 0$ (where the initial data are assigned) and having a *nonvanishing* radius ρ, such that the solutions $\zeta(\tau)$ corresponding to these initial data are *holomorphic* in it, namely for $|\tau| < \rho$ (and note that if $\zeta(\tau)$ is a multicomponent object, the property to be *holomorphic* is featured by each and everyone of its components).

Let us now introduce the following changes of dependent and independent variables:

$$z(t) = \exp(i\lambda\omega t)\zeta(\tau) \qquad [3a]$$

$$\tau \equiv \tau(t) = \frac{\exp(i\omega t) - 1}{i\omega} \qquad [3b]$$

This transformation is called "the trick". The essential part of it is the change of *independent* variable [3b]: and let us re-emphasize that, here and hereafter, the new *independent* variable t is considered as the *real*, "physical time" variable. Note that [3b] entails

$$\tau(0) = 0, \ \dot{\tau}(0) = 1$$

and, most importantly, that $\tau(t)$ is a periodic function of t with period T, see [1]. More specifically, as the time t increases from zero onwards, the complex variable τ travels counterclockwise round and round on the circle C the diameter of which, of length $2/\omega$, lies on the imaginary axis in the complex τ-plane, with one extreme at the origin, $\tau = 0$, and the other at the point $\tau = 2i/\omega$, making a full circle in the time interval T. As for the prefactor $\exp(i\lambda\omega t)$ that multiplies $\zeta(\tau)$ in the right-hand side of [3a], its purpose is to allow, via an appropriate choice of the parameter λ, the deformed system, see below, to have a neater look; however this choice is hereafter restricted by the condition that λ be *real* and *rational*, say

$$\lambda = \frac{p}{q}$$

with p and q two coprime integers and $q > 0$. This restriction is essential to guarantee, via [3], that if $\zeta(\tau)$ is *holomorphic* in τ in the (closed) disk encircled by the circle C, then $z(t)$ is *completely periodic* (namely, each and everyone of its components is *periodic*) with the period

$$\tilde{T} = qT \qquad [4]$$

The deformed dynamical system is the one that obtains from [2] via the trick [3]. It clearly reads as follows:

$$\dot{z} = i\lambda\omega z + \exp[i(\lambda+1)\omega t] \times F\left(\exp(-i\lambda\omega t)z; \frac{\exp(i\omega t)-1}{i\omega}\right) \quad [5]$$

And it is plain, on the basis of the arguments we just gave, that this system is *isochronous*, a sufficient condition for the *complete periodicity* with period $\tilde{T}$, see [4], of its solutions being provided by the inequality

$$\frac{2}{\omega} < \rho$$

which can clearly be satisfied by initial data situated inside an *open* domain of such data, at least provided ω is sufficiently large (actually, in all the examples reported below no restriction on the value of ω is required, namely such an open domain exists for any arbitrary value of $\omega > 0$).

Examples

In this subsection we report tersely several examples of *isochronous* dynamical systems; in each case we also provide the reference where more information can be found. Except when explicitly otherwise mentioned, these dynamical systems are to be considered in the *complex* context.

The first example we report is a Hamiltonian N-body problem which is a generalization of a well-known *integrable* (indeed, *superintegrable*) system (*see* Integrable Systems: Overview). It is characterized by the (normal) Hamiltonian

$$H(\underline{z},\underline{p}) = \frac{1}{2}\sum_{n=1}^{N}(p_n^2+\omega^2 z_n^2) + \frac{1}{4}\sum_{m,n=1;m\neq n}^{N}\sum_{k=1}^{K}\frac{f_{nm}^{(k)}}{k(z_n-z_m)^{2k}} \quad [6a]$$

and correspondingly by the Newtonian equations of motion

$$\ddot{z}_n + \omega^2 z_n = \sum_{m=1,m\neq n}^{N}\sum_{k=1}^{K}\frac{f_{nm}^{(k)}}{(z_n-z_m)^{1+2k}} \quad [6b]$$

Here the $\frac{1}{2}N(N-1)K$ "coupling constants" $f_{nm}^{(k)}$ are arbitrary, except for the symmetry restriction $f_{nm}^{(k)} = f_{mn}^{(k)}$ (see [6a]).

The next example we report is a *real* N-body problem in the horizontal plane, characterized by the Newtonian equations of motions

$$\ddot{\vec{r}}_n = \omega\hat{k}\wedge\dot{\vec{r}}_n + 2\sum_{m=1,m\neq n}^{N}\left(\alpha_{nm}+\beta_{nm}\hat{k}\wedge\right) \times \frac{\left[\dot{\vec{r}}_n\left(\dot{\vec{r}}_m\cdot\vec{r}_{nm}\right)+\dot{\vec{r}}_m\left(\dot{\vec{r}}_n\cdot\vec{r}_{nm}\right)-\vec{r}_{nm}\left(\dot{\vec{r}}_n\cdot\dot{\vec{r}}_m\right)\right]}{r_{nm}^2} \quad [7]$$

Here $\vec{r}_n \equiv (x_n, y_n, 0)$ is a *real* two-vector in the horizontal plane, $\hat{k} \equiv (0,0,1)$ is the unit vector orthogonal to the horizontal plane, the symbol $\wedge$ denotes the (three-dimensional) vector product so that $\hat{k}\wedge\vec{r}_n = (-y_n, x_n, 0)$, and we use the short-hand notation $\vec{r}_{nm} = \vec{r}_n - \vec{r}_m$ entailing $r_{nm}^2 = r_n^2 + r_m^2 - 2\vec{r}_n\cdot\vec{r}_m$. Note that these equations are *translation-* and *rotation-invariant*; and they are *Hamiltonian*, although the corresponding Hamiltonian function is *not* of normal type (kinetic plus potential energy).

The $N(N-1)$ "coupling constants" α_{nm} and β_{nm} are of course real, but they are otherwise *arbitrary* except for the symmetry restrictions $\alpha_{nm} = \alpha_{mn}$, $\beta_{nm} = \beta_{mn}$ which are required in order that this system be *Hamiltonian*. If *all* these coupling constants *vanish*, this dynamical system has a clear physical interpretation: it describes the motion of N equal, electrically charged, point particles, moving in the horizontal plane under the effect of a magnetic field orthogonal to that plane (in the approximation in which the electrostatic interparticle interaction is neglected). In that case each particle moves on a circle, the center and radius of which depend on the initial data, while the time taken to go round it is, in all cases, T, see [1]. If the $\frac{1}{2}N(N-1)$ coupling constants β_{nm} vanish, $\beta_{nm}=0$, and the $\frac{1}{2}N(N-1)$ coupling constants α_{nm} all equal unity, $\alpha_{nm}=1$, the system is a well-known *integrable* (indeed *solvable*) system; and this is as well the case if the $\frac{1}{2}N(N-1)$ coupling constants β_{nm} vanish, $\beta_{nm}=0$, and the $\frac{1}{2}N(N-1)$ coupling constants α_{nm} equal minus one half, and only act among "nearest neighbors", $\alpha_{nm} = -\frac{1}{2}(\delta_{m,n+1}+\delta_{m,n-1})$ (see the entry *Integrable systems* in this Encyclopedia).

Because of its many interesting features as well as the neatness of its equations of motion (especially in their complex version, see below) the honorary title of "goldfish" has been attributed to this model, characterized by the Newtonian equations of motion in the plane [7]. A more detailed discussion of it – in particular of its behavior for initial data *outside* of the region yielding *isochronous* motions – is made in the next section.

Several interesting classes of *isochronous* dynamical systems are reported in Calogero F. (2004b).

We only mention here a remarkably general example, characterized by the Newtonian equations of motion

$$\ddot{\underline{z}} + i\omega\dot{\underline{z}} = \sum_{k=1}^{K} \underline{f}^{(-k)}(\underline{z}, \dot{\underline{z}} + i\omega\underline{z})$$

where $\underline{z} \equiv (z_1, \ldots, z_N)$ is the N-vector whose *complex* components $z_n \equiv z_n(t)$ are the dependent variables, while the "forces" $\underline{f}^{(-k)}(\underline{z}, \tilde{\underline{z}})$ are required to be *analytic* in all their arguments and to satisfy the scaling properties

$$\underline{f}^{(-k)}(\alpha\underline{z}, \tilde{\underline{z}}) = \alpha^{-k}\underline{f}^{(-k)}(\underline{z}, \tilde{\underline{z}})$$

which however entail no restriction on the velocity-dependence of these forces, namely on the dependence of $\underline{f}^{(-k)}(\underline{z}, \tilde{\underline{z}})$ on the (components of the) second, $\tilde{\underline{z}}$, of its two N-vector arguments.

The next example we report is characterized by the Newtonian equations of motion

$$\ddot{\vec{r}}_n + i\omega\dot{\vec{r}}_n + 2\omega^2\vec{r}_n = \sum_{m=1, m\neq n}^{N} \frac{M_m\vec{r}_{mn}}{r_{mn}^3}$$

where we assume the N dependent variables $\vec{r}_n \equiv \vec{r}_n(t)$ to be three-vectors (although the property of *isochronicity* of this deformed system would hold no less if these were S-vectors, with S an arbitrary positive integer) and we use the short-hand notation $\vec{r}_{mn} = \vec{r}_m - \vec{r}_n$. This system is (perhaps) remarkable inasmuch as it represents a (*complex*) deformation of the classical N-body gravitational problem, to which it clearly reduces for $\omega = 0$.

The next example we report is characterized by the following (first-order) equations of motion of oscillator type:

$$\dot{x}_n - ip_n\omega x_n = f_n(\underline{x}, \underline{y}), \; n = 1, \ldots, N$$
$$\dot{y}_m + iq_m\omega y_m = g_m(\underline{x}, \underline{y}), \; m = 1, \ldots, M \qquad [8]$$

Here the N-vector $\underline{x}$, respectively the M-vector $\underline{y}$, have as components the $N + M$ *complex* dependent variables $x_n \equiv x_n(t), y_m \equiv y_m(t)$; the $N + M$ parameters p_n, q_m are all *nonnegative integers* (or they could be *nonnegative rational* numbers); and the $N + M$ *complex* functions f_n, g_m are restricted by the following conditions (which are sufficient to guarantee the *isochronicity* of this dynamical system):

(1) $f_n(\underline{x}, \underline{y})$ and $g_m(\underline{x}, \underline{y})$ are *holomorphic* at $\underline{x} = 0, \underline{y} = 0$;
(2) $\lim_{\varepsilon\to 0}[\varepsilon^{-1}\underline{f}(\varepsilon\underline{x}, \varepsilon\underline{y})] = \underline{0}$, $\lim_{\varepsilon\to 0}[\varepsilon^{-1}\underline{g}(\varepsilon\underline{x}, \varepsilon\underline{y})] = \underline{0}$;
(3) $\underline{f}(\underline{x}, \underline{y})$ and $\underline{g}(\underline{x}, \underline{y})$ are *polynomial* in the y_m;
(4a) $\lim_{\varepsilon\to 0}[\varepsilon^{-1-p_n}f_n(\varepsilon^{\underline{p}}\underline{x}, \varepsilon^{-\underline{q}}\underline{y})] =$ nondivergent, $n = 1, \ldots, N$;
(4b) $\lim_{\varepsilon\to 0}[\varepsilon^{-1+q_m}g_m(\varepsilon^{\underline{p}}\underline{x}, \varepsilon^{-\underline{q}}\underline{y})] =$ nondivergent, $m = 1, \ldots, M$.

In the conditions (4a) and (4b) the notation $\varepsilon^{\underline{p}}\underline{x}$ indicates of course the N-vector of components $\varepsilon^{p_n}x_n$, and likewise $\varepsilon^{-\underline{q}}\underline{y}$ is the M-vector of components $\varepsilon^{-q_m}y_m$.

Note that this dynamical system, [8], includes the *Hamiltonian* case characterized by the restrictions

$$N = M, p_n = q_n, f_n(\underline{x}, \underline{y}) = \frac{\partial V(\underline{x}, \underline{y})}{\partial y_n}, g_n(\underline{x}, \underline{y}) = -\frac{\partial V(\underline{x}, \underline{y})}{\partial x_n}$$

which imply that the equations of motion [8] are just the Hamiltonian equations entailed by the Hamiltonian function

$$H(\underline{x}, \underline{y}) = i\omega\sum_{n=1}^{N} p_n x_n y_n + V(\underline{x}, \underline{y})$$

isochronicity being now guaranteed by the following conditions on the function $V(\underline{x}, \underline{y})$:

(1) $V(\underline{x}, \underline{y})$ is *holomorphic* at $\underline{x} = 0, \underline{y} = 0$;
(2) $\lim_{\varepsilon\to 0}[\varepsilon^{-2}V(\varepsilon\underline{x}, \varepsilon\underline{y})] = \underline{0}$;
(3) $V(\underline{x}, \underline{y})$ is *polynomial* in the y_n;
(4) $\lim_{\varepsilon\to 0}[\varepsilon^{-1}V(\varepsilon^{\underline{p}}\underline{x}, \varepsilon^{-\underline{p}}\underline{y})] =$ nondivergent.

The last two examples we report can be characterized as assemblies of *non-linear harmonic oscillators*, inasmuch as these two dynamical systems (which are actually special cases of more general systems) have the remarkable property that their *generic* solutions (namely, *all* their solutions, except for a lower-dimensional set of *singular* solutions in which one or more of the "moving particles" shoot off to infinity at a finite time) are *completely periodic* with the fixed period T, see [1]. Their Newtonian equations of motion read

$$\ddot{\vec{z}}_{nm} - 3i\omega\dot{\vec{z}}_{nm} - 2\omega^2\vec{z}_{nm} = c\sum_{\nu=1}^{N}\sum_{\mu=1}^{M}\vec{z}_{n\mu}(\vec{z}_{\nu\mu}\cdot\vec{z}_{\nu m})$$

$$\ddot{\vec{z}}_{nm} - 3i\omega\dot{\vec{z}}_{nm} - 2\omega^2\vec{z}_{nm} = c\sum_{\nu=1}^{N}\sum_{\mu=1}^{M}\vec{z}_{\nu\mu}(\vec{z}_{\nu\mu}\cdot\vec{z}_{nm})$$

These are two (different) systems of NM Newtonian equations of motion satisfied by the NM *complex* S-vectors $\vec{z}_{nm}$ (with S an *arbitrary* positive integer); hence here the index n runs from 1 to N, and the index m runs from 1 to M, with N and M two *arbitrary* positive integers, while c is of course an *arbitrary* complex constant (which might actually be rescaled away). The dot sandwiched between two

S-vectors denotes the standard (Euclidian) scalar product, entailing the rotation-invariant character, in S-dimensional space, of these equations of motion. Since these systems only feature *linear* and *cubic* forces, these models are remarkably close to physics; and they become even more applicable if they are written in their *real* versions, that obtain in an obvious manner by setting

$$\vec{z}_{nm} = \vec{x}_{nm} + i\vec{y}_{nm}, c = a + ib$$

In contrast to what we did for the previous examples, let us outline here the derivation of these results. Actually the two systems of Newtonian equations written above are merely special subcases, corresponding to appropriate parametrizations of a square matrix M (of appropriate rank) in terms of S-vectors, of the following nonlinear *matrix* evolution equation:

$$\ddot{M} - 3i\omega\dot{M} - 2\omega^2 M = cM^3 \qquad [9]$$

Hence the findings reported above are merely special cases of the more general result according to which the *generic* solution of this nonlinear *matrix* evolution equation – with $M \equiv M(t)$ a square matrix of *arbitrary* rank – is *periodic* with period T, see [1]:

$$M(t + T) = M(t)$$

And this result is an immediate consequence, via the following *matrix* version of the trick

$$M(t) = \exp(i\omega t)\Psi(\tau), \tau = \frac{\exp(i\omega t) - 1}{i\omega} \qquad [10]$$

of a previous result due to V. I. Inozemtsev, according to which the matrix evolution equation

$$\Psi'' = c\Psi^3$$

which clearly corresponds to [9] via [10], is *integrable* and *all* its solutions $\Psi(\tau)$ are *meromorphic* functions of the independent variable τ.

The Transition to Deterministic Chaos

In this section we illustrate, using the *real* N-body problem in the plane characterized by the Newtonian equations of motion [7], the behavior of an *isochronous* system of the kind described above when the initial data fall *outside* of the region yielding *isochronous* motions.

To do this it is convenient to use the *complex* version of the equations of motion [7], that obtain from [7] by setting

$$z_n = x_n + iy_n, \vec{r}_n = (x_n, y_n, 0), \quad \hat{k} = (0, 0, 1), a_{nm} = \alpha_{nm} + i\beta_{nm} \qquad [11]$$

and read as follows:

$$\ddot{z}_n = i\omega\dot{z}_n + 2\sum_{m=1, m\neq n}^{N} \frac{a_{nm}\dot{z}_n\dot{z}_m}{z_n - z_m} \qquad [12]$$

The main tool of our analysis is the (particularly simple) version of the trick appropriate to this model,

$$z_n(t) = \zeta_n(\tau), \tau = \frac{\exp(i\omega t) - 1}{i\omega} \qquad [13a]$$

entailing

$$z_n(0 = \zeta_n(0), \dot{z}_n(0) = \zeta_n'(0) \qquad [13b]$$

that relates our equations of motion [12] to the equations of motion

$$\zeta_n'' = 2\sum_{m=1, m\neq n}^{N} \frac{a_{nm}\zeta_n'\zeta_m'}{\zeta_n - \zeta_m} \qquad [14]$$

These equations of motion, together with the initial data $\zeta_n(0), \zeta_n'(0)$ (see [13b]) define the solutions $\zeta_n \equiv \zeta_n(\tau)$ in the *complex* τ-plane. The "physical" evolution of the points $z_n \equiv z_n(t)$ as functions of the *real* time variable t is then given by the evolution of the corresponding coordinates $\zeta_n(\tau)$, see [13a], as the *complex* variable τ travels round and round on the circle C in the *complex* τ-plane, the diameter of which of length $2/\omega$, has one extreme at the origin $\tau = 0$ and the other on the positive imaginary axis at $\tau = 2i/\omega$. It is therefore clear that the behavior of $z_n(t)$ as a function of the *real*, "physical time" variable t depends on the analytic structure of $\zeta_n(\tau)$ as function of the *complex* variable τ, in particular of the singularities, if any, of this function $\zeta_n(\tau)$ that fall in the disk D encircled by the circle C in the *complex* τ-plane.

Let us tersely review the relevant analysis. We recall first of all that (it can be proven that) there exists in phase space an *open* region of initial data $z_n(0), \dot{z}_n(0)$, characterized by *large* values of the moduli $|z_n(0) - z_m(0)|$ of the initial interparticle distances and by *small* values of the moduli of the initial particle velocities $|\dot{z}_n(0)|$ (see [14] and [13b]), that guarantees (all components $\zeta_n(\tau)$ of) the corresponding solution $\underline{\zeta}(\tau)$ of [14] to be *holomorphic* in (a disk of radius ρ centered at the origin $\tau = 0$ of the *complex* τ-plane that includes) the circle C, hence the corresponding solution $\underline{z}(t)$ to be *completely periodic* with period T, see [13a] and [1]. This result guarantees the *isochronous* character of this model, [12], for any arbitrarily given assignment of the coupling constants a_{nm}.

Next, let us restrict, for simplicity, our consideration to models [12] in which the coupling constants a_{nm} are *real* and *nonnegative*,

$$a_{nm} \geq 0 \qquad [15]$$

Then the singularities of the generic solution $\underline{\zeta}(\tau)$ of [14] – which occur at values τ_b of τ where *two* coordinates $\zeta_n(\tau)$ coincide, say $\zeta_\mu(\tau_b) = \zeta_\nu(\tau_b) = b$ (see the right-hand side of [14]) – are *branch points* characterized by the exponent, say,

$$\gamma = \gamma_{\mu\nu} = \frac{1}{1 + a_{\mu\nu}} \qquad [16]$$

so that in their neighborhood, namely for $\tau \approx \tau_b$,

$$\zeta_s(\tau) = b \pm c(\tau - \tau_b)^\gamma + v(\tau - \tau_b) + \sum_{k=1}^{\infty} \sum_{\ell,m=0 \, \ell+m\geq 1}^{\infty} \varphi^{(s)}_{k\ell m}(\tau - \tau_b)^{k+\ell\gamma+m(1-\gamma)}$$

$$s = \mu, \nu \qquad [17a]$$

$$\zeta_n(\tau) = b_n + v_n(\tau - \tau_b) + \sum_{k=1}^{\infty} \sum_{\ell=\delta_{k1}}^{\infty} \sum_{m=0}^{\infty} \varphi^{(n)}_{k\ell m}(\tau - \tau_b)^{k+\ell\gamma+m(1-\gamma)}$$

$$n \neq \mu, \nu \qquad [17b]$$

The $\pm$ sign in front of c in the right- hand side of the first, [17a], of these formulas indicates that one sign must be chosen for $s = \mu$, the opposite for $s = \nu$. Note that here the $4 + 2(N - 2) = 2N$ constants $\tau_b, b, c, v, b_n, v_n$ are *a priori* arbitrary – except for the obvious restrictions $b_n \neq b, b_n \neq b_m$ – while the coefficients $\varphi^{(s)}_{k\ell m}, \varphi^{(n)}_{k\ell m}$ can be computed from these constants, recursively, by inserting this *ansatz*, [17], in the equations of motion [14]. The fact that the number, $2N$, of *a priori* undetermined coupling constants equals the number of arbitrary initial data for this system of ODEs, [14], indicates that this kind of branch points, characterized by the exponents γ_{nm}, see [16], is the typical singularity featured by the generic solution $\underline{\zeta}(\tau)$ of [14]. (Branch points with different exponents may appear, but only in *nongeneric* solutions $\underline{\zeta}(\tau)$ which, at some value τ_b of τ, feature the coincidence of more than two components, say $\zeta_\mu(\tau_b) = \zeta_\nu(\tau_b) = \zeta_\lambda(\tau_b)$).

We conclude therefore that the *generic* solution $\underline{\zeta}(\tau)$ of [14] features a, generally infinite, number of branch points, that generally affect each of its components $\zeta_n(\tau)$, and which are characterized, for the class of models to which we are restricting attention here, see [15]) by (*real*) exponents γ_{nm}, see [16], which are then clearly characterized by the inequalities

$$0 < \gamma_{nm} \leq 1$$

What does this tell us about the *generic* solution $\underline{z}(t)$ of the equations of motions of primary interest to us, [12], in particular about its evolution as function of the *real* "time" variable t?

To the solution $\underline{\zeta}(\tau)$ is associated a Riemann surface the structure of which is determined by the character and distribution of the branch points of $\underline{\zeta}(\tau)$ in the complex τ-plane (each of which is generally featured by each component $\zeta_n(\tau)$ of $\underline{\zeta}(\tau)$, although generally not in the same way: see [17]), and we know from [13a] that the values taken by $\underline{z}(t)$ as t evolves from $t = 0$ towards $t = \infty$ coincide with the values taken by $\underline{\zeta}(\tau)$ as the independent variable τ travels, on that Riemann surface associated with $\underline{\zeta}(\tau)$, counterclockwise round and round on the circle C defined above (the diameter of which lies on the imaginary axis in the complex τ-plane, with one end at $\tau = 0$ and the other at $\tau = 2i/\omega$), employing a period T, see [1], to make each full round. Hence the behavior of the solution $\underline{z}(t)$ of [12] depends on the structure of the Riemann surface associated with the corresponding solution $\underline{\zeta}(\tau)$ of [14], and specifically on the number of different sheets of that surface that are visited as one travels on it before returning, if ever, to the main sheet from which the travel started at $t = \tau = 0$.

If no other sheet is visited besides the main one, the corresponding solution $\underline{z}(t)$ is of course periodic with period T, see [1] and [13a],

$$\underline{z}(t + T) = \underline{z}(t) \qquad [18]$$

This happens provided no branch point is featured by $\underline{\zeta}(\tau)$ on its main sheet *inside* the circle C; and, as already indicated above, it has been proven (even in the more general case with arbitrary coupling constants a_{nm}) that there is an *open* region having full dimensionality in the phase space of initial data, see [13b], that yields such an outcome, implying the *isochronicity* of the model characterized by the Newtonian equations of motion [12]. This region R of initial data has a boundary – a lower-dimensional domain in the phase space of initial data – out of which emerge motions leading, at a time t_b smaller than T, to a "particle collision", say $z_\nu(t_b) = z_\mu(t_b)$.

The character of the solution $\underline{z}(t)$ yielded by initial data *outside* of the region R depends on the structure of the Riemann surface associated with the corresponding solution $\underline{\zeta}(\tau)$. This is mainly determined by the values of the branch point exponents γ_{nm}, which are themselves determined by the values of the coupling constants a_{nm}, see [17] and [16]. Let us focus on the (more interesting) case in which these constants a_{nm} are *rational* numbers, entailing that the coefficients γ_{nm} determining the

character of the branch points are as well *rational*, see [16], so that each of the cuts associated with them opens the way, in the Riemann surface, to a *finite* number of sheets. There are then two possibilities, each generally characterized by *open* regions of initial data having full dimensionality in phase space, the boundaries of which always are (lower-dimensional) domains out of which emerge motions leading, in a time t_b smaller than T, to a "particle collision".

One possibility is that the number B of sheets visited before returning to the main sheet be *finite*, $B < \infty$; the corresponding solutions $\underline{z}(t)$ are then *completely periodic* with period $\tilde{T} = (B+1)T$, $\underline{z}(t+\tilde{T}) = \underline{z}(t)$.

Another possibility is that the number of new sheets visited be *unlimited*, namely that the structure of the Riemann surface be such that, by traveling round and round on it along the circle C one *never* returns back to the main sheet. This can happen, even if the exponents γ_{nm} are *all rational* so that via the cuts associated to each of them access is gained to only a *finite* number of new sheets, because of the possibility that an *infinity* of branch points be located inside the circle C on the *infinite* sheets associated to these branch points, via a never ending mechanism of branch points nesting. Whenever this happens the corresponding solution $\underline{z}(t)$ is *aperiodic*; and it is moreover likely that it then be *chaotic*, in the sense of displaying a *sensitive dependence* on its initial data. Indeed this will happen whenever some ones out of this infinity of branch points fall arbitrarily close to the contour C, because then a *minute* change in the initial data, to which there will correspond a *minute* change in the pattern of these branch points of $\underline{\zeta}(\tau)$ in the complex τ-plane, will cause some relevant branch point to cross over from outside the circle C to inside it, or viceversa, and this will eventually affect quite significantly the time evolution of $\underline{z}(t)$, by causing a change in the sequence of sheets that get visited by traveling along the circle C on the Riemann surface associated to the corresponding $\underline{\zeta}(\tau)$.

This phenomenology has a clear "physical interpretation", which can be qualitatively understood as follows. The N-body problem characterized by the Newtonian equations of motion [12] generally yields confined motions, the trajectory of each particle tending to wind round and round – it would indeed reduce to a circle were it not for the interaction with the other particles. A possibility, as we know, is that this N-body motion be *completely periodic*, with the same period T that characterizes the circular motion of each particle when the two-body interparticle interaction is altogether missing ($a_{nm} = 0$). Another possibility, in the case discussed above with *rational* coupling constants, is that there exist other motions which are as well *completely periodic*, but with periods which are *integer multiples* of T. A third possibility, which cannot *a priori* be excluded, is that there also exist motions which are *aperiodic* but in some way overall *ordered*, perhaps featuring trajectories that eventually wind up around *limit cycles*. And still another possibility is that the motions described by the solution $\underline{z}(t)$ be *aperiodic* and *disordered*. In this case the physical mechanism causing a sensitive dependence on the initial data can be understood as follows. Such disordered motions necessarily feature *near misses*, in which, typically, two particles pass *quite close* to each other (while the probability that an actual collision occur among *point particles* moving *in a plane* is of course *a priori* nil). Such a *near miss* in the motion described by $\underline{z}(t)$ corresponds – see the discussion above – to a branch point of the corresponding solution $\underline{\zeta}(\tau)$ occurring *quite close* to the circle C in the complex τ-plane (which is the one-dimensional region of the two-dimensional complex τ-plane in which the values of $\underline{\zeta}(\tau)$ correspond to the values $\underline{z}(t)$ describing the motion of physical particles moving as functions of the time t); and in the generic case of a *two-body* near miss, there is a correspondence between the fact that such a branch point occur *just inside*, or *just outside*, the circle C, and the way the particles pass, on one or the other side, by each other. Likewise, the tiny change in the initial data that causes, in the context of the solutions $\underline{\zeta}(\tau)$ – see the discussion above – a branch point of $\underline{\zeta}(\tau)$ to pass from inside to outside the circle C, or viceversa, corresponds, in the context of the "physical" solutions $\underline{z}(t)$, to a change occurring in the corresponding *near miss*, from the case in which the two particles involved in it slide by each other on one side to the case in which they instead slide by each other on the other side – entailing a significant change in the subsequent motion (indeed, the closer a near miss, the more it affects the motion, due to the singularity of the two-body interaction at zero separation, see [12]).

The phenomenology outlined here does indeed occur in this goldfish model. It also occurs – rather similarly if more simply, since in this case only square-root branch points occur, irrespective of the values of the coupling constants – in the model [6] with $K = 1$. Indeed, it is clear that this phenomenology provides a paradigm of rather general applicability for the transition from *isochronicity* to *deterministic chaos*, indeed perhaps for the generic *onset* of *deterministic chaos*.

See also: Bifurcations of Periodic Orbits; Calogero–Moser–Sutherland Systems of Nonrelativistic and Relativistic Type; Integrable Systems: Overview; Quantum Calogero–Moser Systems; Synchronization of Chaos.

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Isomonodromic Deformations

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Introduction

In this article we consider families of linear differential equations whose monodromy data do not depend on the parameters. Such families are called isomonodromic deformations of any of the equations of the family (for the definitions of a regular and Fuchsian linear system and of their monodromy groups, see Riemann–Hilbert Problem).

Schlesinger's Equation

The best-studied example of an isomonodromic deformation is the Fuchsian system on Riemann's sphere $CP^1 = \mathbf{C} \cup \infty$ considered by L Schlesinger:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \left(\sum_{j=1}^{p+1} \frac{A_j}{t - a_j}\right) X \qquad [1]$$

Here the poles $a_j \in \mathbf{C}$ are free parameters and the matrices-residua A_j depend analytically on $a := (a_1, \ldots, a_{p+1})$; therefore, system [1] is in fact a family of linear systems which is an analytic deformation of the system obtained for $a_j = a_j^0$.

One can think of system [1] as defined by the Pfaffian system

$$\mathrm{d}X = \omega_s X, \quad \omega_s = \sum_{j=1}^{p+1} \frac{A_j}{t - a_j} \mathrm{d}(t - a_j) \qquad [2]$$

Suppose first that the poles a_j vary within small nonintersecting disks of the points a_j^0, so small that the standard system of generators of the monodromy group could be defined by one and the same contours for all values of the parameters a_j (see **Figure 1** from Riemann–Hilbert Problem). Suppose also that one chooses ∞ as base point and that one has

$$X|_{t=\infty} = I \qquad [3]$$

(where I is the identity matrix) for all values of the parameters a_j. Finally, suppose that all matrices A_j are nonresonant, that is, without two eigenvalues differing by a nonzero integer. Then the following conditions are necessary and sufficient for system [1] to be isomonodromic:

$$\mathrm{d}A_i(a) = -\sum_{j=1, j\neq i}^{p+1} \frac{[A_i(a), A_j(a)]}{a_i - a_j} \mathrm{d}(a_i - a_j)$$
$$i = 1, \ldots, p+1 \qquad [4]$$

This system (called Schlesinger's equations) results from the Frobenius integrability condition $\mathrm{d}\omega_s = \omega_s \wedge \omega_s$ of system [2].

Remarks 1

(i) To find the matrices-residua A_j as functions of a and given their values $A_j|_{a=a^0}$ is a Cauchy problem. It is solvable for a close to a^0 and the matrices A_j are analytic in a.

(ii) The differential of A_i being a commutator $[A_i, .]$, the matrix A_i remains within its conjugacy class throughout the deformation.

(iii) Schlesinger's equations are the necessary and sufficient conditions for isomonodromy also in the case when system [1] has a logarithmic pole at ∞ whose matrix-residuum does not change throughout the deformation. In this case the solution to system [1] in its Levelt's decomposition at ∞ (*see* Riemann–Hilbert Problem) equals $U_\infty(1/t)t^{-D_\infty}t^{-E_\infty}G$, where D_∞ is a diagonal matrix with integer entries, E_∞ is an upper-triangular constant matrix, and U_∞ is holomorphic at ∞ and such that $U_\infty(0) = I$.

Definition 2 The deformation satisfying condition [4] with initial condition [3] for the solution to system [1] is called the normalized Schlesinger deformation.

Remark 3 When the matrices-residua A_j are nonresonant, then every isomonodromic deformation of system [1] with $a_j = a_j^0$ is either the normalized Schlesinger deformation or is a nonnormalized Schlesinger deformation, that is, obtained from the normalized one by a change of variables $X \mapsto C(a)X, C(a) \in GL(n, C)$. In this way, one has $X|_{t=\infty} = C(a)$ instead of [3] and the deformation is described by a Pfaffian system with a form of the kind $\omega_n = \omega_s + \sum_{j=1}^{p+1} \gamma_j(a)\mathrm{d}a_j$.

Example 4 The following one-parameter Fuchsian family is an isomonodromic Schlesinger deformation:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \left(\sum_{j=1}^{p+1} \frac{A_j}{t - ba_j^0}\right)X$$

Here the matrices A_j are constant and the parameter b takes nonzero values. Indeed, one either checks directly that there holds condition [4] or one makes the change of time (which does not change monodromy) $t \mapsto bt$ after which the parameter b disappears.

A A Bolibrukh has shown that in the resonant case every isomonodromic deformation of a Fuchsian system is described by an integrable Pfaffian system with 1-form $\omega = \omega_n + \omega_m$, where the meromorphic 1-form ω_m vanishes at ∞ and has poles of orders $\leq r_j$ along the hyperplanes $\{x - a_j = 0\}$; here r_j is the largest nonzero integer difference between two eigenvalues of the matrix A_j.

Consider now Schlesinger's equation in the global situation, that is, when the poles a_j belong to the universal covering Z of the space $C^n \backslash \Delta$, where Δ is the "diagonal," that is, the union of all sets $\{a_i = a_j\}$, $i \neq j$. Suppose that the matrices A_j are nonresonant. There are values of a (their set is denoted by Θ) for which some entries of some of the matrices-residua A_j tend to ∞. Typically, at such points the matrices A_j have poles of second order; this is a result due to Bolibrukh. Indeed, set $A_j = Q_j^{-1} J_j Q_j$, where J_j is the Jordan normal form of A_j; hence, this is a constant matrix; we assume that $Q_j \in SL(n, C)$. Typically, at points of Θ the matrices Q_j and Q_j^{-1} have simple poles, which makes a pole of second order for A_j.

B Malgrange and, independently, T Miwa have proved that system [4] is completely integrable and that it has the Painlevé property: "The only movable singularities of its solutions are poles." (The fixed singularities of the solutions are, by definition, along the points of Z which are over Δ. The positions of the movable singularities depend on the initial condition, that is, on the values of the matrices A_j for $a = a^0$.) In other words, the solutions to Schlesinger's equation are matrices meromorphic on Z.

Theorem 5 *The set* Θ *of movable singular points of the Schlesinger equation is the set of zeros of a function* τ *(the Miwa* τ*-function) holomorphic on* Z *and such that*

$$\frac{1}{2}\sum_{i,j,i\neq j} \frac{\mathrm{tr}(A_i(a)A_j(a))\mathrm{d}(a_i - a_j)}{a_i - a_j} = \mathrm{d}\log(\tau(a))$$

Some improvements of this result are due to Malgrange and Bolibrukh.

Isomonodromy and Confluence

The idea to consider a linear system of ordinary differential equations with a pole of order higher than 1 as embedded into a family of Fuchsian systems with confluence of the poles has been proposed by V I Arnol'd in 1984 and independently by J-P Ramis in 1988. The idea has been used by A Duval, B Khesin, A A Glutsyuk, and other authors. In particular, it is interesting to relate the Stokes multipliers (defined in the next section) of the system obtained as a result of a confluence to the monodromy groups of the

Fuchsian systems obtained for values of the parameters before the confluence occurs.

Example 6 Consider the one-parameter family of linear systems:

$$(t^2-\lambda)\mathrm{d}X/\mathrm{d}t=(A(\lambda)t+B(\lambda))X \qquad [5]$$

Here the matrices A, B, and X are $n\times n$. Suppose that $t\in\mathbf{C}$ (i.e., we do not consider singularity at ∞), $\lambda\in(\mathbf{C},0)$. Then for $\lambda\neq 0$ the system is Fuchsian – it has two logarithmic poles at $\pm\lambda^{1/2}$ whose confluence for $\lambda=0$ gives as a result a pole at 0 which might be of order 2 if $B(0)\neq 0$ or 1 if $B(0)=0$.

In this section we consider only the situation when the family producing the confluence is isomonodromic for values of the parameters before the confluence.

Example 7 This is the case of family [5] with $B\sim 0$ and A being a constant nonresonant $n\times n$ matrix. Indeed, the change of time $t\mapsto\lambda^{1/2}t(*)$ transforms the family into the family $(t^2-1)\mathrm{d}X/\mathrm{d}t=tAX$ (independent of λ) which is a Fuchsian system (at ∞ as well).

Suppose now that $t\in CP^1$ (i.e., we consider the singularity at ∞ as well). Hence, the monodromy operator M_∞ around ∞ is independent of λ up to conjugacy (it is conjugate to $\exp(-2\pi\mathrm{i}A)$). On the other hand, consider the monodromy operator M' defined by a contour circumventing counterclockwise both poles at $\pm\lambda^{1/2}$ (one can choose as such a contour a circumference centered at the origin and of sufficiently large radius). It equals M_∞^{-1}, and it is well defined for $\lambda=0$ as well. (This is not the case of the monodromy operators defined by contours circumventing only one of the poles at $\pm\lambda^{1/2}$.) Hence, up to conjugacy M' is independent of λ. As M' is in a sense the only monodromy operator that can be defined by a contour depending continuously on λ for all $\lambda\in(\mathbf{C},0)$ and not passing through a pole of the system, one can say that the family is strongly isomonodromic.

Example 8 Consider now family [5] with $n=2$,

$$A=\begin{pmatrix} d & 0\\ 0 & d\end{pmatrix},\qquad B=\begin{pmatrix} 0 & \lambda\\ 0 & 0\end{pmatrix}$$

where $d\in\mathbf{C}$. For $\lambda\neq 0$ the family is isomonodromic – the change of time $(*)$ followed by the change of variables

$$X\mapsto\begin{pmatrix}\lambda^{1/2} & 0\\ 0 & 1\end{pmatrix}X(**)$$

brings the family to the form

$$(t^2-1)\frac{\mathrm{d}X}{\mathrm{d}t}=\left(\begin{pmatrix} d & 0\\ 0 & d\end{pmatrix}t+\begin{pmatrix} 0 & 1\\ 0 & 0\end{pmatrix}\right)X$$

which is independent of λ, hence, isomonodromic. However, the change of variables $(**)$ is not defined for $\lambda=0$. The monodromy operator M' (defined as above) is scalar for $\lambda=0$ and conjugate to a Jordan block of size 2 for $\lambda\neq 0$. Hence, the family is not strongly isomonodromic.

The following example is closely connected to singularity theory. It has been suggested by F Pham.

Example 9 Consider the Abelian integrals

$$I_1=\int \mathrm{d}x/(x^3+sx+t)\quad\text{and}$$
$$I_2=\int x\,\mathrm{d}x/(x^3+sx+t)$$

taken over a closed contour γ belonging to a nonsingular fiber of the function $f(x)=x^3+sx+t$. Suppose that $x^3+sx+t\neq 0$ on γ. Obviously, I_1 and I_2 depend only on $[\gamma]$, the class of homotopy equivalence of γ. Set

$$x^3+sx+t=(x-x_1)(x-x_2)(x-x_3),$$
$$x_j=x_j(s,t)$$

Then one has

$$I_k=2\pi\mathrm{i}\sum_{j=1}^{3}\delta_{k,j}x_j^{k-1}\Big/\left(3x_j^2+s\right),\quad k=1,2$$

where the integers $\delta_{k,j}$ depend only on $[\gamma]$ (the contour γ is homotopy equivalent to a linear combination with integer coefficients of small loops around the roots of f; the integral along such a loop is computed using residua). Note that

$$\dot{x}_j:=\mathrm{d}x_j/\mathrm{d}t=-1\Big/\left(3x_j^2+s\right)$$

An easy computation shows that the integrals I_1,I_2 satisfy the following Picard–Fuchs system of differential equations:

$$-t\dot{I}_1-2s\dot{I}_2/3=2I_1/3$$
$$2s^2\dot{I}_1/9-t\dot{I}_2=I_2/3$$

The system admits also a presentation of the form

$$\left(t^2+\frac{4s^3}{27}\right)\begin{pmatrix}\dot{I}_1\\ \dot{I}_2\end{pmatrix}=\begin{pmatrix}-2t/3 & 2s/9\\ -4s^2/27 & -t/3\end{pmatrix}\begin{pmatrix}I_1\\ I_2\end{pmatrix}$$

Here the unknown variables form a vector column of length 2; to obtain a 2×2 matrix, one has to choose another contour γ' (linearly independent

with γ as a linear combination of the loops around the roots x_i) which gives the second column of the matrix. The system is strongly isomonodromic – its matrix-residuum at ∞ equals diag(2/3, 1/3); hence, the monodromy operator M' up to conjugacy equals $\mathrm{diag}(\exp(-4\pi i/3), \exp(-2\pi i/3))$.

A A Bolibrukh has considered the possibility of confluence of poles in Schlesinger's equation (i.e., the possibility to have equalities of the form $a_i = a_j$ in system [1]). He has considered the so-called normalized isomonodromic confluences, that is, isomonodromic confluences defined by Pfaffian systems with coefficient forms $\omega = \omega_s + \omega_m$ alone (see the previous section). He has shown that a normalized isomonodromic confluence of singular points of Fuchsian systems of linear differential equations on Riemann's sphere can only lead to a system with regular singular points. This is a partial answer to a problem stated by V I Arnol'd: how to express a system with regular singular points as a limit of Fuchsian systems?

Other Results

In the case of a linear system with irregular singular point, isomonodromy means that the formal monodromy and the Stokes multipliers do not change throughout the deformation. The formal monodromy can be computed from the formal normal form (the latter can be found algorithmically; this is due to H Turrittin). Consider, for simplicity, the nonresonant case, that is, the case when the leading matrix in the Laurent series of the system at the singular point has distinct eigenvalues (this definition differs from the one in the case of a Fuchsian singular point). The Stokes multipliers are linear operators acting on the solution space. They are defined as follows: there exist sectors of maximal opening centered at the singular point on each of which the solution is uniquely defined by its asymptotic development. Two solutions X_1, X_2 having one and the same asymptotic development in two overlapping sectors are related by $X_1 = X_2 C$, where C is a Stokes multiplier. The monodromy operator is expressed as a product of the operator of formal monodromy and the Stokes multipliers. Isomonodromic deformations of systems with irregular singular points have been constructed by B Malgrange. Isomonodromic deformations have been used by Y Sibuya and C H Lin and by Y Sibuya and T J Tabara to investigate Stokes multipliers.

At the beginning of the twentieth century, P Painlevé and B Gambier have classified the differential equations of second order,

$$u_{xx} = R(x, u, u_x) \qquad [6]$$

(where R is analytic in x and rational in u and u_x) whose solutions do not have branch-type movable singularities. From the 50 equations (up to local transformation) discovered by them only six are not reduced to linear ones. These are the so-called Painlevé equations. They appear often as isomonodromy conditions for families of linear differential equations and this has given the idea to develop the isomonodromic deformation method. It consists in associating with eqn [6] a linear system

$$\mathrm{d}\Psi/\mathrm{d}\lambda = A(\lambda, x, u, u_x)\Psi \qquad [7]$$

with matrix-valued coefficients rational in λ. The deformation of the coefficients in x is described by eqn [6] in such a way that the monodromy data of system [7] remain the same. Thus, the monodromy data of system [7] are first integrals of eqn [6].

Example 10 The Painlevé II equation

$$u_{xx} - xu - 2u^3 = \nu$$

is associated with the system

$$\frac{\mathrm{d}\Psi}{\mathrm{d}\lambda} = \begin{pmatrix} -4i\lambda^2 - ix - 2iu^2 & 4i\lambda u - 2u_x - \dfrac{i\nu}{\lambda} \\ -4i\lambda u - 2u_x + \dfrac{i\nu}{\lambda} & 4i\lambda^2 + ix + 2iu^2 \end{pmatrix} \Psi$$

The idea to present the Painlevé equations as isomonodromy conditions originate from the works of Fuchs (1907) and Garnier (1912). It has been used, for example, in the papers of Flaschka and Newell (1980), Jimbo and Miwa (1981), and Its and Novokshenov (1986).

See also: Holonomic Quantum Fields; Integrable Systems: Overview; Painlevé Equations; Riemann–Hilbert Problem; WDVV Equations and Frobenius Manifolds.

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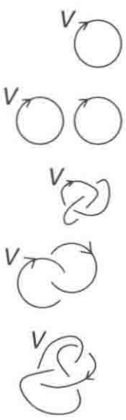
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The Jones Polynomial

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Introduction

A "link" is a finite family of disjoint, smooth, oriented or unoriented, closed curves in $\mathbb{R}^3$ or equivalently S^3. A "knot" is a link with one component. The "Jones polynomial" $V_L(t)$ is a Laurent polynomial in the variable $\sqrt{t}$ which is defined for every oriented link L but depends on that link only up to orientation-preserving diffeomorphism, or equivalently isotopy, of $\mathbb{R}^3$. Links can be represented by diagrams in the plane and the Jones polynomials of the simplest links are given below.



$= 1$

$= -\left(\frac{1}{\sqrt{t}} + \sqrt{t}\right)$

$= t + t^3 - t^4$

$= -\sqrt{t}\,(1 + t^2)$

$= \frac{1}{t^2} - \frac{1}{t} + 1 - t + t^2$

The Jones polynomial of a knot (and generally a link with an odd number of components) is a Laurent polynomial in t.

The most elementary ways to calculate $V_L(t)$ use the "linear skein theory" ideas of Conway (1970). Indeed, it is not hard to see by induction that $V_L(t)$ is defined by its invariance under isotopy, the normalization $V_{\bigcirc}(t) = 1$ and the skein formula

$$\frac{1}{t} V_{L_+} - tV_{L_-} = \left(\sqrt{t} - \frac{1}{\sqrt{t}}\right) V_{L_0}$$

which holds for any three oriented links having diagrams which are identical except near one crossing where they differ as below.



As such the Jones polynomial resembles the Alexander (1928) polynomial $\Delta_L(t)$ which can be calculated in exactly the same manner as $V_L(t)$ except that the skein relation becomes

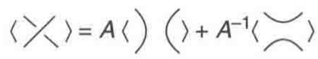
$$\Delta_{L_+} - \Delta_{L_-} = \left(\sqrt{t} - \frac{1}{\sqrt{t}}\right) \Delta_{L_0}$$

A two-variable generalization P_L of both Δ_L and V_L, sometimes called the HOMFLYPT polynomial, was found in Freyd *et al.* (1985) and Przytycki and Traczyk (1988). It satisfies the most general skein relation

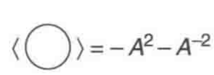
$$xP_{L_+} + yP_{L_-} + zP_{L_0} = 0$$

for homogeneous variables x, y, and z.

The other skein-like definition of V_L was found in Kauffman (1987). Begin with unoriented link diagrams up to planar istotopy. The Kauffman bracket $\langle L \rangle$ of such a diagram is calculated using

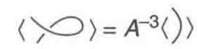


where the $\langle \cdot \rangle$ notation means that the relation may be applied to that part of the link diagrams inside the bracket, the rest of the diagrams being identical. If $\langle L \rangle$ were to be an invariant of three-dimensional isotopy it is easy to see that



$= -A^2 - A^{-2}$

which further implies



Thus, $\langle L \rangle$ cannot be a three-dimensional isotopy invariant as such. However, if L is given an

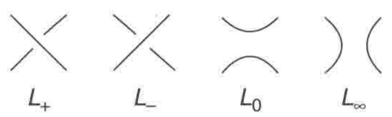
orientation (then called $\vec{L}$), a simple renormalization solves the problem and it is true that

$$(*) \qquad V_L(A^4) = A^{-3\,\mathrm{writhe}(\vec{L})}\langle L\rangle$$

where writhe ($\vec{L}$) is the sum over the crossings of L of $+1$ for a positive crossing (⤫) and -1 for a negative crossing (⤫).

The formula $(*)$ is readily proved by induction but a more structural proof will be discussed later on, connected with physics. If the crossings in a link alternate between over and under as one follows the string around, the highest and lowest degree terms in the Kauffman bracket can readily be located. This led to the proof of some old conjectures about alternating knots in Murasugi (1987), Kauffman (1987), and Thistlethwaite (1987).

The Kauffman two-variable polynomial $F_L(a,x)$ is defined in Kauffman (1990) by considering the linear skein relation involving all four possibilities at a crossing:

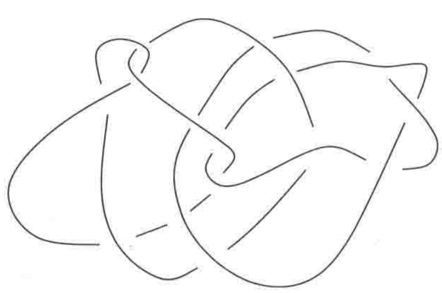


This polynomial contains $V_L(T)$ as a specialization but not the Alexander polynomial.

The above polynomials are quite powerful at distinguishing links one from another, including links from their mirror images, which corresponds for the Jones polynomial to replacing t by t^{-1}. More power can be added to the polynomials if simple geometric operations are allowed. "Cabling" entails replacing a single strand with several parallel copies and the polynomials of cables of a link are also isotopy invariants if attention is paid to the writhe of a diagram.

The following problem, however, is open at the time of writing this article: "Does there exist a knot in $\mathbb{R}^3$, different from the unknot ○, whose Jones polynomial is equal to 1?"

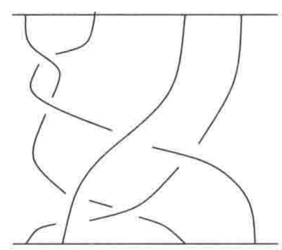
For links with more than one component, it is known (Thistlethwaite 2001, Eliahou *et al.* 2003) that the answer to the corresponding question is yes, the simplest example being:



One of the reasons that the question above has not been answered is presumably that, unlike with the Alexander polynomial, we have little intuitive understanding of the meaning of the "t" in $V_L(t)$. Perhaps, the most promising theory in this context is in Khovanov (2000) where a complex is constructed whose Euler characteristic, in an appropriately graded sense, is the Jones polynomial. The homology of the complex is a finer invariant of links known as "Khovanov homology."

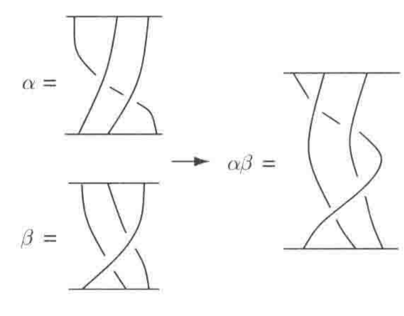
Braids

A braid (see Birman (1974)) on n strings is a collection of curves in $\mathbb{R}^3$ joining n points in a horizontal plane to the n points directly below them on another horizontal plane. If the endpoints of the braid are on a straight line, the braid can be drawn as in the example below (where $n = 4$).

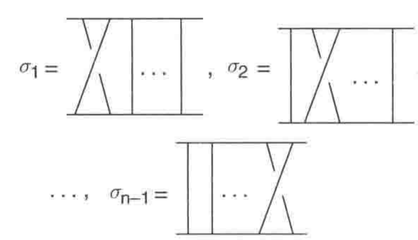


The crucial property of a braid is that the tangent vector to the curves can never be horizontal. Braids are considered up to isotopies which are supported between the top and bottom planes.

Braids on n strings form a group, called B_n, under concatenation (plus some isotopy) as below:



Let $\sigma_1, \sigma_2, \ldots, \sigma_{n-1}$ be the braids below:



Artin's presentation (Birman 1974) of the braid group is on the generators $\sigma_1, \sigma_2, \ldots, \sigma_{n-1}$ with the relations

$$\begin{aligned} \sigma_i\sigma_{i+1}\sigma_i &= \sigma_{i+1}\sigma_i\sigma_{i+1} \quad &&\text{for } 1 \le i \le n-2 \\ \sigma_i\sigma_j &= \sigma_j\sigma_i &&\text{if } |i-j| \ge 2 \end{aligned}$$

Thus, to find linear representations of B_n, it suffices to find matrices $\rho_1, \rho_2, \ldots, \rho_{n-1}$ satisfying the above relations (with σ replaced by ρ). One such representation (of dimension n) called the (nonreduced) Burau representation is given by the row-stochastic matrices

$$\rho_1 = \begin{pmatrix} 1-t & t & 0 & 0 & \ldots \\ 1 & 0 & 0 & 0 & \ldots \\ 0 & 0 & 1 & 0 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}$$

$$\rho_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots \\ 0 & 1-t & t & 0 & \ldots \\ 0 & 1 & 0 & 0 & \ldots \\ 0 & 0 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}, \quad \ldots$$

$$\ldots, \quad \rho_{n-1} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & 1-t & t \\ 0 & \ldots & 1 & 0 \end{pmatrix}$$

This representation is known not to be faithful for $n \ge 5$ but faithful for $n \le 3$. The case $n = 4$ remains open. (See Moody (1991), Long and Paton (1993), and Bigelow (1999)).

Braids can be viewed in several ways, which lead to several generalizations. For instance, identifying the vertical axis for a braid with time and taking the intersection of horizontal planes with the braids shows that elements of B_n can be thought of as motions of n distinct points in the plane. Thus, it is natural that

$$B_n \cong \pi_1(\{\mathbb{C}^n \backslash \Delta\}/S^n)$$

when Δ is the set $\{(z_1, \ldots, z_n) | z_i = z_j \text{ for some } i \ne j\}$ and the symmetric group S_n acts freely on $\mathbb{C}^n \backslash \Delta$ by permuting coordinates. But Δ is the zero-set of the frequently encountered function

$$\prod_{i<j} (z_i - z_j)$$

so the braid group may naturally be generalized as the fundamental group of $\mathbb{C}^n$ minus the singular set of some algebraic function (Birman 1974). Or, motions of points can be extended to motions of the whole plane and a braid defines a diffeomorphism of the plane minus n points. Thus, the braid group may be generalized as the "mapping class group" of a surface with marked points (Birman 1974).

The Temperley–Lieb Algebra

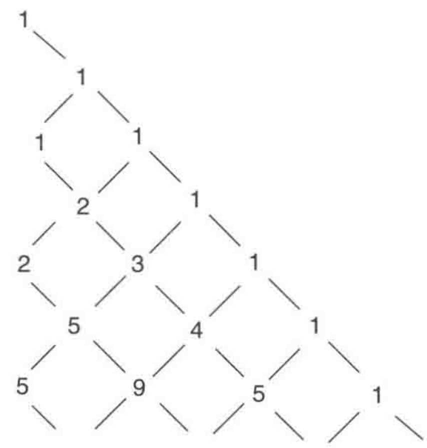
If $\tau \in \mathbb{C}$ one may define the algebra $TL(n, \tau)$ with identity 1 and generators $e_1, e_2, \ldots, e_{n-1}$ subject to the following relations:

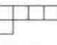
$$\begin{aligned} e_i^2 &= e_i \\ e_i e_{i\pm1} e_i &= \tau e_i \\ e_i e_j &= e_j e_i \quad \text{if } |i-j| \ge 2 \end{aligned}$$

Counting reduced words on the e_i's shows that

$$\dim\{TL(n, \tau)\} \le \frac{1}{n+1}\binom{2n}{n}$$

and in Jones (1983) it is shown that these numbers, the Catalan numbers, are indeed the dimensions of the Temperley–Lieb algebras. In the obvious way, $TL(n, \tau) \subseteq TL(n+1, \tau)$. If τ^{-1} is not in the set $\{4\cos^2 q\pi; q \in \mathbb{Q}\}, TL(n, \tau)$ is semisimple and its structure is given by the following Bratteli diagram:



where the integers on each row are the dimensions of the irreducible representations of $TL(n, \tau)$ and the diagonal lines give the restriction of representations of $TL(n, \tau)$ to $TL(n-1, \tau)$. These representations are naturally indexed by Young diagrams with n boxes and at most two rows:  with the diagonal lines in the Bratteli diagram corresponding to removal/addition of a box. The dimension of the representation corresponding to the diagram whose second row has r boxes ($r \le n$) is

$$\binom{n}{r} - \binom{n}{r-1}$$

One may attempt to make $TL(n,\tau)$ into a C^*-algebra and look for Hilbert space representations (with $e_i \neq 0$), by imposing $e_i^* = e_i$. From (Wenzl 1987), this is only possible (for all n) when

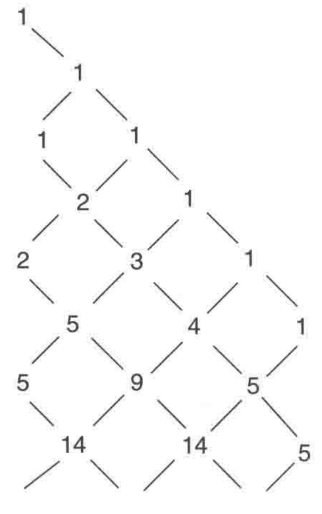
1. $\tau \in \mathbb{R}$, $0 < \tau \leq 1/4$, or
2. $\tau^{-1} \in \{4\cos^2 \pi/m, m = 3, 4, 5, \dots\}$.

The proof uses the fact that f_n, inductively defined by

$$f_{n+1} = f_n - \frac{[2]_q[n+1]_q}{[n+2]_q} f_n e_{n+1} f_n$$

must be an orthogonal projection with $e_i f_n = f_n e_i = 0$ for $i \leq n$. These f_n are sometimes called Jones–Wenzl idempotents. (Here $\tau^{-1} = 2 + q^2 + q^{-2}$ and for this and later formulas we define the quantum integer $[n]_q = (q^n - q^{-n})/(q - q^{-1})$).

When $\tau^{-1} = 4\cos^2(\pi/m)$, the Hilbert space representations decompose according to Bratteli diagrams obtained by truncating – eliminating the 1 on the mth row, and all representations below and to the right of it, so that for $m = 7$ we would obtain



In terms of Young diagrams, this corresponds to only taking those diagrams whose row lengths differ by at most $m - 2$. The existence of these Hilbert space representations is from Jones (1983).

The Temperley–Lieb algebras arose in Jones (1983) as orthogonal projections onto subfactors of II_1 factors. As such the Hilbert space structure was manifest. The trace on a II_1 factor also yielded a trace on the $TL(n,\tau)$.

To be precise, there is for each m a unique linear map $\mathrm{tr}: TL(n,\tau) \to \mathbb{C}$ with:

1. $\mathrm{tr}(1) = 1$
2. $\mathrm{tr}(ab) = \mathrm{tr}(ba)$
3. $\mathrm{tr}(xe_{n+1}) = \tau\,\mathrm{tr}(x)$ for $x \in TL(n+1,\tau)$.

This trace may be calculated either from (1), (2), and (3), or using the representations, as a weighted sum of ordinary matrix traces. The weight for the representation of $TL(n,\tau)$, the second row of whose Young diagram has r boxes, is

$$\frac{[n-r+1]_q}{([2]_q)^n}$$

Thus, if $x \in TL(n,\tau)$ and π_r is the $\binom{n}{r} - \binom{n}{r-1}$ dimensional irreducible representation, then

$$\mathrm{tr}(x) = \frac{1}{(q+q^{-1})^n} \sum_{r=0}^{[n/2]} [n-r+1]_q \,\mathrm{trace}\,(\pi_r(x))$$

One also has

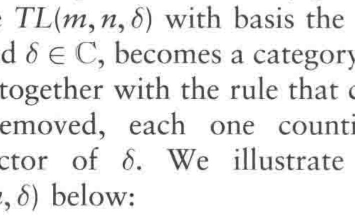
$$\mathrm{tr}(f_n) = \frac{[n+2]_q}{([2]_q)^{n+1}}$$

so that the disappearance of the "1" from the Bratteli diagram is mirrored by the vanishing of the trace of the corresponding projection.

Positivity of tr, $\mathrm{tr}(a^*a) \geq 0$, is responsible for all the Hilbert space structures. To explicitly construct the Hilbert space representations, one may use the GNS construction: take the quotient of the $*$-algebra by the kernel of the form $\langle a, b\rangle = \mathrm{tr}(b^*a)$ which makes this quotient a Hilbert space on which $TL(n,\tau)$ will act with the e_i's as orthogonal projections. Explicit bases can be obtained easily if desired, using paths on the Bratteli diagram, or Young tableaux.

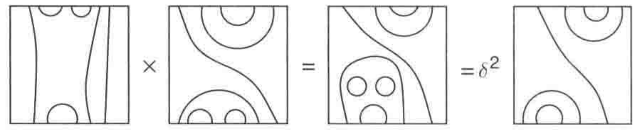
A useful diagrammatic presentation of $TL(n,\tau)$ was discovered in Kauffman (1987). A (Kauffman) TL diagram (for non-negative integers m and n) is a rectangle with n marked points on the top and m on the bottom with nonintersecting smooth curves inside the rectangle connecting the boundary points as illustrated below.

A (5, 7)-diagram

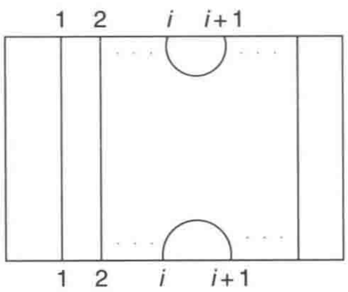


Two Kauffman TL diagrams are considered the same if they connect the same pairs of boundary points.

The vector space $TL(m,n,\delta)$ with basis the set of (m,n) diagrams, and $\delta \in \mathbb{C}$, becomes a category with this concatenation together with the rule that closed curves may be removed, each one counting a (multiplicative) factor of δ. We illustrate their product in $TL(m,n,\delta)$ below:

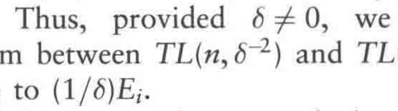


Of special interest is the algebra $TL(n, n, \delta)$. If we define E_i to be the diagram below:



then $E_i^2 = \delta E_i$, $E_iE_{i\pm1}E_i = E_i$, and $E_iE_j = E_jE_i$ for $|i-j| \geq 2$. Thus, provided $\delta \neq 0$, we have an isomorphism between $TL(n, \delta^{-2})$ and $TL(n, n, \delta)$ by mapping e_i to $(1/\delta)E_i$.

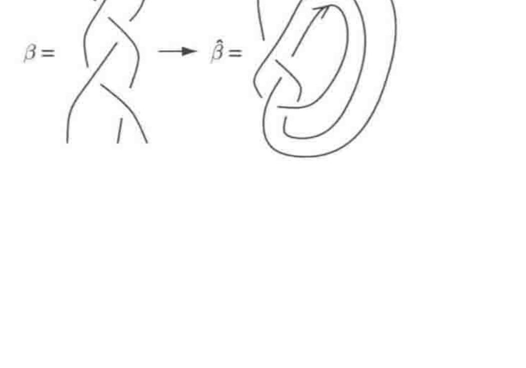
One of the nicest features of the Kauffman diagrams is that they yield simple explicit bases for the irreducible representations. To see this, call a curve in a diagram a "through-string" if it connects the top of the rectangle to the bottom. Then all (m, n) diagrams are filtered by the number of through-strings and if we let $TL(m, n, k, \delta)$ be the span of (m, n) diagrams with at most k through-strings, we have $TL(k, n, \delta)TL(n, m, k, \delta) \subseteq TL(k, m, k, \delta)$. Thus, $V_{n,m} = TL(n, m, m, \delta)/TL(n, m, m-1, \delta)$ is a $TL(n, \delta^{-2})$-module, a basis of which is given by (m, n)-diagrams with m through-strings $(m \leq n)$. The number of such diagrams is $\binom{n}{m} - \binom{n}{m-1}$ and it follows from Jones (1983) that all these representations are irreducible for "generic" δ (i.e., $\delta \notin \{2\cos \mathbb{Q}\pi\}$) and that they may be identified with those indexed by Young diagrams as below:



The invariant inner product on $V_{n,m}$ is defined by $\langle v, w \rangle = w^*v$ for the natural identification of $V_{m,m}$ with $\mathbb{C}$ (* is the obvious involution from (m, n) diagrams to (n, m) diagrams.).

The Original Definition of $V_L(t)$

Given a braid $\beta \in B_n$ one may form an oriented link $\hat{\beta}$ called the closure of β by tying the top of the braid to the bottom as illustrated below:



All oriented links occur in this way (Birman 1974) but if $\alpha \in B_n$, $\alpha\beta\alpha^{-1}$ and $\beta\sigma_n^{\pm1}$ (in B_{n+1}) have the same closure.

Theorem 1 (Markov) (*Birman 1974*). *Let $\sim$ be the equivalence relation on $\coprod_{n=1}^{\infty} B_n$ (all braids on any number of strings) generated by the two "moves" $\beta \sim \beta\sigma_n^{\pm1}$ and $\beta \sim \alpha\beta\alpha^{-1}$. Then $\beta_1 \sim \beta_2$ if and only if the links $\hat{\beta}_1$ and $\hat{\beta}_2$ are the same.*

It is easily checked that, if $1, e_1, e_2, e_3, \ldots$ satisfy the TL relations of the section "The Temperley–Lieb algebra," then sending σ_i to $(t+1)e_i - 1$ (with $\tau^{-1} = 2 + t + t^{-1}$) defines a representation ρ_n of B_n inside $TL(n, \tau)$ for each n. The representation is unitary for the C*-algebra structure when $\tau^{-1} = 4\cos^2 \pi/n$, $n = 3, 4, 5, \ldots$ (and $t = e^{\pm 2\pi i/n}$). It is an open question whether ρ_n is faithful for all n. It contains the Burau representation as a direct summand.

Combining the properties of the trace tr defined on TL with Markov's theorem, one obtains immediately that, for $\alpha \in B_n$, the following function of t depends only on $\hat{\alpha}$:

$$\left(-\sqrt{t} - \frac{1}{\sqrt{t}}\right)^{n-1} \sqrt{t}^{\,-e} \mathrm{tr}(\rho_n(\alpha))$$

(here $e \in \mathbb{Z}$ is the "exponent sum" of α as a word on $\sigma_1, \sigma_2, \ldots, \sigma_{n-1}$).

A simple check using the (oriented) skein-theoretic definition of the Jones polynomial shows that this function of t is precisely $V_{\hat{\alpha}}(t)$. This is how $V_L(t)$ was first discovered in Jones (1985).

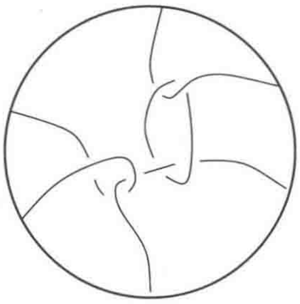
Although less elementary, this approach to $V_L(t)$ does have some advantages. Let us mention a few.

1. One may use representation theory to do calculations. For instance, using the weighted sum of ordinary traces to calculate tr as in the section "The Temperley–Lieb algebra," one obtains readily the Jones polynomial of a torus knot (i.e., $\hat{\alpha}$ where $\alpha = (\sigma_1\sigma_2 \cdots \sigma_{p-1})^q \in B_p$ if p and q are relatively prime). It is

$$\frac{t^{(p-1)(q-1)/2}}{1-t^2}(1 - t^{p+1} - t^{q+1} - t^{p+q})$$

2. If one restricts attention to links realizable as $\hat{\alpha}$ for $\alpha \in B_n$ for fixed n, the computation of $V_{\hat{\alpha}}(t)$ can be performed in polynomial time as a function of the number of crossings in $\hat{\alpha}$. Thus, one has computational access to rather complicated families of links.
3. Unitarity of the representation when $t = e^{\pm\frac{2\pi i}{n}}$ can be used to bound the size of $|V_L(t)|$. For instance, if $\alpha \in B_k$ and $V_{\hat{\alpha}}(t) = (-\sqrt{t} - (1/\sqrt{t}))^{k-1}$, then α is in the kernel of ρ_n, and $|V_{\hat{\beta}}(e^{\pm 2\pi i/n})| \leq (2\cos \pi/n)^{k-1}$ for any other $\beta \in B_k$.

The representation of the braid group inside the TL algebra should be thought of as an extension of the Jones polynomial to "special knots with boundary." The coefficients of the words in the e_i's (or equivalently the Kauffman TL diagrams) are all invariants of the braid. We can further remove the braid restriction and consider arbitrary knots and links with boundary, known as "tangles" (Conway 1970).



Tangles may be oriented or not and their invariants may be evaluated either by reduction to a system of elementary tangles using skein relations or by organizing the tangle and representing it in an algebra. See Turaev (1994).

A similar algebraic approach is available for the HOMFLYPT and Kauffman two-variable polynomials. The algebra playing the role of the TL algebra is the Hecke algebra for HOMFLYPT (Freyd *et al.* 1985, Jones 1987) and the BMW algebra (Birman and Wenzl 1989, Murakami 1990) for the Kauffman polynomial. The BMW algebra was discovered after the Kauffman polynomial in order to provide an analog of the TL and Hecke algebras. For detailed analysis of the Hilbert space and other structures for both Hecke and BMW algebras, see Wenzl (1988) and Wenzl (1990).

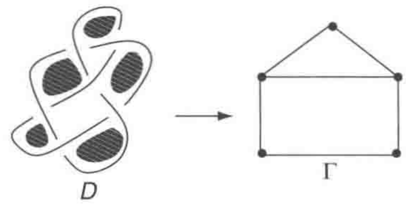
Connections with Statistical Mechanics

One might say that turning a knot into a braid organizes the knot by "putting it on a lattice," thereby creating a physical model with the crossings of the knot as interactions. Taking the trace of the braid is evaluating the partition function with periodic (vertical) boundary conditions.

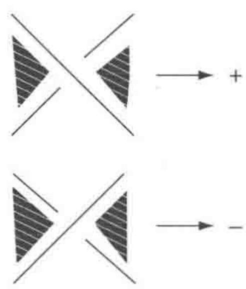
This is more than wishful thinking. The Temperley–Lieb algebra arose from transfer matrices in both the Potts and ice-type models in two dimensions (Temperley and Lieb 1971) and each "e_i" implements the addition of one more interaction to the system. (The same e_i's as in the ice-type models were rediscovered in the subfactor context in Pimsner and Popa (1986)). Thus, the Jones polynomial of a closed braid is the partition function for a statistical mechanical model on the braid. In Jones (1983), it is observed that knowledge of the Jones polynomial for a family of links called French sinnets would constitute a solution of the Potts model in two dimensions.

In Temperley and Lieb (1971), the TL relations are used to establish the mathematical equivalence of the Potts and ice-type (six-vertex) models. In Baxter (1982, chapter 12), this equivalence is shown for Potts models on an arbitrary planar graph. In view of this, it is not surprising that statistical mechanical models can be defined directly on link diagrams to give explicit formulas for $V_L(t)$ (and other invariants) as partition functions. This works most easily for the Q-state Potts model.

Given an unoriented link diagram D, shade the regions of the plane black and white and form the planar graph Γ whose vertices are the black regions and whose edges are the crossings as below:



Assign + and − to each edge according to the following scheme:



Fix $Q \in \mathbb{N}$ and two symmetric matrices $w_\pm(a, b)$ for $1 \leq a, b \leq Q$. The partition function of the diagram is then

$$Z_D = \sum_{\text{states}} \prod_{\text{edges of } \Gamma} w_\pm(\sigma, \sigma')$$

where a "state" is a function from the vertices of Γ to $\{1, 2, \ldots, Q\}$ and, given an edge of Γ and a state, σ and σ' denote the values of the state at the ends of that edge (w_+ and w_- are used according to the sign of the edge).

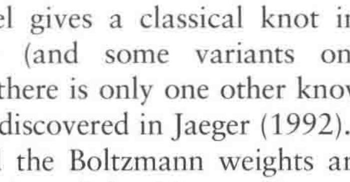
The "Potts model" is defined by the property that the "Boltzmann weights" $w_\pm(\sigma, \sigma')$ depend only on whether $\sigma = \sigma'$ or not. It is a miracle that the choice (with $Q = 2 + t + t^{-1}$)

$$w_\pm(\sigma, \sigma') = \begin{cases} t^{\pm 1} & \text{if } \sigma = \sigma' \\ -1 & \text{otherwise} \end{cases}$$

gives the Jones polynomial of the link defined by D as its partition function (up to a simple normalization). See Jones (1989) for details.

It is natural to look for other choices of $w_\pm$ which give knot invariants. The Fateev–Zamolodchikov (1982) model gives a classical knot invariant but besides that (and some variants on the Jones polynomial) there is only one other known choice of any interest, discovered in Jaeger (1992). In this case, $Q = 100$ and the Boltzmann weights are symmetric under the action of the Higman–Sims group on the Higman–Sims graph with 100 vertices. The knot invariant is a special value of the Kauffman two-variable polynomial.

The other side of Temperley–Lieb equivalence is the "ice-type" model which is a "vertex model." That is to say the "spins" reside on the edges of a graph and the interactions occur at the vertices. To use vertex models in knot theory, the knot projection D itself is the (4-valent) graph. The ice-type model has two spin states per edge so that a state of the system is a function from the edges of the graph to the set $\{\pm\}$; the Boltzmann weights are given by two 4×4 matrices $w_\pm(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ where the σ's are ± 1 and w_+ and w_- are the contributions of



to the partition function, respectively. Furthermore, we may think of a state as a locally constant function σ on D so for any $f : \{\pm 1\} \to \mathbb{R}$ we may form the term $\int_D f(\sigma)\mathrm{d}\theta$ corresponding to interaction with an external field ($\mathrm{d}\theta$ is the curvature or change of angle form on D). Then the partition function is

$$Z_D = \sum_{\text{states}} \left(\prod_{\text{crossings of } D} w_\pm(\sigma_1, \sigma_2, \sigma_3, \sigma_4) \right) \mathrm{e}^{\int_D f(\sigma)\mathrm{d}\theta}$$

A (nonphysical) specialization of the six-vertex model yields values of f and $w_\pm$ for which Z_D is a link invariant equal to $V_L(t)$. See Jones (1989).

As with the Potts model, one may try to generalize to more general $w_\pm$ and f. This is much more successful for these "vertex" models than it was for models like the Potts model. The theory of quantum groups (Jimbo 1986, Drinfeld 1987, Rosso 1988) allows one to obtain link invariants (as partition functions for vertex models) for each simple finite-dimensional Lie algebra $\mathfrak{A}$ and each assignment of an irreducible representation of $\mathfrak{A}$ to the components of the link. The images of the braid generators σ_i in the corresponding braid group representations are called "R-matrices." It is the Yang–Baxter equation that gives isotopy invariance of the partition function. In this way, one obtains (by an infinite family of one-variable specializations) the HOMFLYPT polynomial (sl_n) and the Kauffman polynomial (orthogonal and symplectic algebras) and more polynomials. The geometric operation of cabling corresponds to the tensor product of representations.

Connections with Quantum Field Theory

Conformal Field Theory

If φ is a (multicomponent) field in one chiral half of a two-dimensional conformal field theory (CFT), the correlation functions

$$\langle \varphi(z_1)\varphi(z_2)\cdots\varphi(z_n)\rangle$$

(where $z_i \in \mathbb{C}$) are expected to be singular if $z_i = z_j$ for some $i \neq j$, holomorphic otherwise and satisfy a linear differential equation. Thus, analytic continuation should determine a unitary monodromy representation of $\pi_1(\mathbb{C}^n \backslash \{(z_1, z_2, \ldots, z_n) | z_i = z_j \text{ for some } i \neq j\})$ on the vector space of solutions to the differential equation near a point. In Tsuchiya and Kanie (1988), these representations were calculated for the SU(2) WZW (Wess–Zumino–Witten) model, where the differential equation is known as the Khniznik–Zamolodchikov equation. The corresponding braid group representations were shown to be those obtained in the section "The original definition of $V_L(t)$" and cablings thereof.

Topological Quantum Field Theory

In Witten (1989), the following formula appears:

$$\begin{aligned} &V_L(\mathrm{e}^{2\pi \mathrm{i}/(k+2)}) \\ &\quad = \int_A \exp\left\{\frac{i}{\hbar}\int_{S^3} \mathrm{tr}(A \wedge \mathrm{d}A + 2/3\, A \wedge A \wedge A)\right\} \\ &\quad \times \prod_j \mathrm{tr}\left(\mathrm{Pexp} \oint_j A\right)[\mathfrak{D}A] \end{aligned}$$

where A ranges over all functions from S^3 to the Lie algebra su(2), modulo the action of the gauge group SU(2). Also $\hbar = \pi/k$ and j runs over the components of the link L, to each of which is assigned an irreducible representation of SU(2). Parallel transport around a component j using A yields the linear map $\mathrm{Pexp}\oint_j A$ whose trace is constant modulo gauge transformations. And $[\mathfrak{D}A]$ is a fictitious diffeomorphism invariant measure on all A's modulo gauge transformation.

There are at least two ways to interpret this formula.

1. As a solvable topological quantum field theory (TQFT) in $2+1$ dimensions, according to Witten (1988) and Atiyah (1988, 1989). One is then obliged to expand the context and conclude that $V_L(e^{2\pi i/n})$ is defined for (possibly empty) links in an arbitrary 3-manifold. The TQFT axioms then provide an explicit formula for the invariant if the 3-manifold is obtained from surgery on a link. In particular, the invariant of a 3-manifold without a link is a statistical mechanics type sum over assignments of irreducible representations of SU(2) to the components of the surgery link. The key condition making this sum finite is that only representations up to a certain dimension (determined by n) are allowed. This is the vanishing of the Jones–Wenzl idempotent of the section "The Temperley–Lieb algebra." This explicit formula was rigourously shown to be a manifold invariant in Reshetikhin and Turaev (1991). For a more simple treatment, see Lickorish (1997) and for the whole TQFT treatment, see Blanchet *et al.* (1995).
2. As a perturbative QFT. The stationary-phase Feynman diagram technique may be applied to obtain the coefficients of the expansion of Witten's formula in powers of $\hbar$ or equivalently $1/n$. These coefficients are known to be "finite type" or Vassiliev invariants and have expressions as integrals over configurations of points on the link, see Vassiliev (1990) and Bar-Natan (1995).

Algebraic Quantum Field Theory

In the Haag–Kastler operator algebraic framework of quantum field theory (Haag 1996), statistics of quantum systems were interpreted in Doplicher *et al.* (1971, 1974) (DHR) in terms of certain representations of the symmetric group corresponding to permuting regions of spacetime. To obtain the symmetric group, the dimension of spacetime needs to be sufficiently large. It was proposed in Fredenhagen *et al.* (1989) that the DHR theory should also work in low dimensions with the braid group replacing the symmetric group, and that unitary braid group representations defined above should be the ones occurring in quantum field theory. The "statistical dimension" of the DHR theory turns up as the square root of the index of a subfactor (this connection was clearly established in Longo (1989, 1980)). The mathematical issue of the existence of quantum fields with braid statistics was established in Wassermann (1998) using the language of loop group representations. Actual physical systems with nonabelian braid statistics have not yet been found but have been proposed in Freedman (2003) as a mechanism for quantum computing.

Acknowledgments

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See also: Braided and Modular Tensor Categories; C^*-Algebras and their Classification; Hopf Algebras and *q*-Deformation Quantum Groups; Knot Homologies; Knot Invariants and Quantum Gravity; Knot Theory and Physics; Large-*N* and Topological Strings; Mathematical Knot Theory; Schwarz-Type Topological Quantum Field Theory; String Field Theory; Topological Knot Theory and Macroscopic Physics; Topological Quantum Field Theory: Overview; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory; von Neumann Algebras: Subfactor Theory; Yang–Baxter Equations.

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Kac–Moody Lie Algebras *see* Solitons and Kac–Moody Lie Algebras

KAM Theory and Celestial Mechanics

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Introduction

Kolmogorov–Arnol'd–Moser (KAM) theory deals with the construction of quasiperiodic trajectories in nearly integrable Hamiltonian systems and it was motivated by classical problems in celestial mechanics such as the n-body problem. Notwithstanding the formidable bulk of results, ideas and techniques produced by the founders of the modern theory of dynamical systems, most notably by H Poincaré and G D Birkhoff, the fundamental question about the persistence under small perturbations of invariant tori of an integrable Hamiltonian system remained completely open until 1954. In that year, A N Kolmogorov stated what is now usually referred to as the KAM theorem (in the real-analytic setting) and gave a precise outline of its proof, presenting a strikingly new and powerful method to overcome the so-called small-divisor problem (resonances in Hamiltonian dynamics produce, in the perturbation series, divisors which may become arbitrarily small, making convergence argument extremely delicate). Subsequently, KAM theory has been extended and applied to a large variety of different problems, including infinite-dimensional dynamical systems and partial differential equations with Hamiltonian structure. However, establishing the existence of quasiperiodic motions in the n-body problem turned out to be a longer story, which only very recently has reached a satisfactory level; the point being that the n-body problems present strong degeneracies, which violate the main hypotheses of the KAM theorem.

This article gives an account of the ideas and results concerning the construction of quasiperiodic solutions in the planetary n-body problem. The synopsis of the article is the following.

The next section gives the analytical description of the planetary $(1+n)$-body problem.

In the subsection "Kolmogorov's theorem and the RPC3BP (1954)," original version of the KAM theorem is recalled, giving an outline of its proof and showing its implications for the simplest many-body case, namely, the restricted, planar, and circular three-body problem.

In the section "Arnol'd's theorem," the existence of a positive measure set of initial data in phase space giving rise to quasiperiodic motions near coplanar and nearly circular unperturbed Keplerian trajectories is presented. The rest of the section is devoted to the proof of Arnol'd's theorem following the historical developments: Arnol'd's proof (1963a) for the planar three-body case is presented, the extension to the spatial three-body case due to Laskar and Robutel (1995) is discussed, and Herman's proof – in the form given by Féjoz in 2004 – of the general spatial $(1+n)$-case is presented.

In the section "Lower dimensional tori," a brief discussion of the construction of lower-dimensional elliptic tori bifurcating from the Keplerian unperturbed motions is given (these results have been established in the early 2000s).

Finally, the problem of taking into account real astronomical parameter values is considered and a recent result on an application of (computer-assisted) KAM techniques to the solar subsystem formed by Sun, Jupiter, and the asteroid Victoria is briefly mentioned.

The Planetary $(1+n)$-Body Problem

The evolution of $(1+n)$-body systems (assimilated to point masses) interacting only through gravitational attraction is governed by Newton's equations.

If $u^{(i)} \in \mathbb{R}^3$ denotes the position of the ith body in a given reference frame and if m_i denotes its mass, then Newton's equations read

$$\frac{d^2 u^{(i)}}{dt^2} = -\sum_{\substack{0\leq j\leq n \\ j\neq i}} m_j \frac{u^{(i)} - u^{(j)}}{|u^{(i)} - u^{(j)}|^3}, \quad i = 0, 1, \ldots, n \quad [1]$$

Here the gravitational constant is taken to be equal to 1 (which amounts to rescale the time t). Equations [1] are equivalent to the standard Hamilton's equations corresponding to the Hamiltonian function

$$\mathcal{H}_{\text{New}} := \sum_{i=0}^{n} \frac{|U^{(i)}|^2}{2m_i} - \sum_{0\leq i<j\leq n} \frac{m_i m_j}{|u^{(i)} - u^{(j)}|} \quad [2]$$

where $(U^{(i)}, u^{(i)})$ are standard symplectic variables and the phase space is the "collisionless domain" $\widehat{\mathcal{M}} := \{U^{(i)}, u^{(i)} \in \mathbb{R}^3\colon u^{(i)} \neq u^{(j)}, 0 \leq i \neq j \leq n\}$; the symplectic form is the standard one: $\sum_i dU^{(i)} \wedge du^{(i)} := \sum_{i,k} dU_k^{(i)} \wedge du_k^{(i)}$; $|\cdot|$ denotes the standard Euclidean norm. Introducing the symplectic coordinate change $(U, u) = \phi_{\text{hel}}(R, r)$,

$$\phi_{\text{hel}}: \begin{cases} u^{(0)} = r^{(0)}, \quad u^{(i)} = r^{(0)} + r^{(i)} \quad (i = 1, \ldots, n) \\ U^{(0)} = R^{(0)} - \sum_{i=1}^{n} R^{(i)}, \quad U^{(i)} = R^{(i)} \\ (i = 1, \ldots, n) \end{cases} \quad [3]$$

one sees that the Hamiltonian $\mathcal{H}_{\text{hel}} := \mathcal{H}_{\text{New}} \circ \phi_{\text{hel}}$ does not depend upon $r^{(0)}$ (recall that a local diffeomorphism is called symplectic if it preserves the symplectic form). This means that $R^{(0)}$ ($\equiv$ total linear momentum) is a global integral of motion. Without loss of generality, one can restrict attention to the invariant manifold $\mathcal{M}_0 := \{R^{(0)} = 0\}$ (invariance of eqn [1] by changes of inertial reference frames).

In the "planetary" case, one assumes that one of the bodies, say $i = 0$ (the Sun), has mass much larger than that of the other bodies (this accounts for the index "hel," which stands for "heliocentric"). To make the perturbative character of the problem transparent, one may introduce the following rescalings. Let

$$m_i = \varepsilon \bar{m}_i, \quad X^{(i)} = \frac{R^{(i)}}{\varepsilon m_0^{5/3}}, \quad x^{(i)} = \frac{r^{(i)}}{m_0^{2/3}}$$
$$(i = 1, \ldots, n) \quad [4]$$

and rescale time by a factor $\varepsilon m_0^{7/3}$ (which amounts to dividing the new Hamiltonian by such a factor); then, the flow of the Hamiltonian $\mathcal{H}_{\text{hel}}$ on $\mathcal{M}_0$ is equivalent to the flow of the Hamiltonian

$$\mathcal{H}_{\text{plt}} := \sum_{i=1}^{n} \left(\frac{|X^{(i)}|^2}{2\mu_i} - \frac{\mu_i M_i}{|x^{(i)}|} \right) + \varepsilon \sum_{1\leq i<j\leq n} \left(X^{(i)} \cdot X^{(j)} - \frac{\bar{m}_i \bar{m}_j / m_0^2}{|x^{(i)} - x^{(j)}|} \right) \quad [5]$$

on the phase space $\mathcal{M} := \{X^{(i)}, x^{(i)} \in \mathbb{R}^3\colon 1 \leq i \leq n$ and $0 \neq x^{(i)} \neq x^{(j)}\}$ with respect to the standard symplectic form $\sum_{i=1}^{n} dX^{(i)} \wedge dx^{(i)}$; the mass parameters are defined as

$$M_i := 1 + \varepsilon \frac{\bar{m}_i}{m_0}, \qquad \mu_i := \frac{\bar{m}_i}{m_0 + \varepsilon \bar{m}_i} = \frac{\bar{m}_i}{m_0} \frac{1}{M_i} \quad [6]$$

The following observations can be made:

1. The Hamiltonian

   $$\mathcal{H}_{\text{plt}}^{(0)} := \sum_{i=1}^{n} \left(\frac{|X^{(i)}|^2}{2\mu_i} - \frac{\mu_i M_i}{|x^{(i)}|} \right)$$

   is integrable and represents the sum of n two-body systems formed by the Sun and the ith planet (disregarding the interaction with the other planets).
2. The transformation ϕ_{hel} in eqn [3] preserves the total angular momentum $\widehat{C} := \sum_{i=0}^{n} U^{(i)} \times u^{(i)}$, which is a vector-valued integral for $\mathcal{H}_{\text{New}}$. Thus, the three components, C_k, of $C := \sum_{i=1}^{n} X^{(i)} \times x^{(i)}$ (which is proportional to $\widehat{C}$ and is termed the "total angular momentum"), are integrals for $\mathcal{H}_{\text{plt}}$. The integrals C_k do not commute: if $\{\cdot,\cdot\}$ denotes the standard Poisson bracket, then $\{C_1, C_2\} = C_3$ (and, cyclically, $\{C_2, C_3\} = C_1, \{C_3, C_1\} = C_2$). Nevertheless, one can form two (independent) commuting integrals, for example, $|C|^2$ and C_3. This shows that the (spatial) $(1 + n)$-body problem has $(3n - 2)$ degrees of freedom.
3. An important special case is the planar $(1 + n)$-body problem. In such a case, one assumes that all the "single" angular momenta $C^{(i)} := X^{(i)} \times x^{(i)}$ are parallel. In this case, the motion takes place on a fixed plane orthogonal to C and (up to a rotation of the reference frame) one can take, as symplectic variables, $X^{(i)}, x^{(i)} \in \mathbb{R}^2$. The Hamiltonian $\mathcal{H}_{\text{pln}}$ governing the dynamics of the planar $(1 + n)$-body problem is, then, given on the right-hand side of eqn [5] with $X^{(i)}$, $x^{(i)} \in \mathbb{R}^2$. Notice that the planar $(1 + n)$-body problem has $2n$ degrees of freedom.
4. For a deeper understanding of the perturbation theory of the planetary many-body problem, it is necessary to find "good" sets of symplectic coordinates, which the founders of celestial

mechanics (most notably, Jacobi, Delaunay, and Poincaré) have done. In particular, Delaunay introduced an analytic set of symplectic "action-angle" variables. Recall the Delaunay variables for the two-body "reduced Hamiltonian"

$$\mathcal{H}_{\rm Kep} = \frac{|X|^2}{2\mu} - \frac{\mu M}{|x|}$$

Let $\{k_1, k_2, k_3\}$ be a standard orthonormal basis in the x-configuration space; let the angular momentum $C = X \times x$ be nonparallel to k_3 and let the energy $E = \mathcal{H}_{\rm Kep} < 0$. In such a case, $x(t)$ describes an ellipse lying in the plane orthogonal to C, with focus in the origin and fixed symmetry axes. Let a be the semimajor axis of the ellipse spanned by x; $\imath$ (the inclination) be the angle between k_3 and C; $G = |C|$; $\Theta = G \cos \imath = C \cdot k_3$; $L = m\sqrt{Ma}$; ℓ be the mean anomaly of x ($:= 2\pi$ times the normalized area spanned by x measured from the perihelion P, which is the point of the ellipse closest to the origin); θ be the angle between k_1 and $N := k_3 \times C$ ($:=$ oriented "node"); and g be the argument of the perihelion ($:=$ the angle between N and (O, P)). Then (letting $\mathbb{T} := \mathbb{R}/(2\pi\mathbb{Z})$)

$$\begin{aligned} &(L, G, \Theta) \in \{L > 0\} \times \{G > \Theta > 0\} \\ &(\ell, g, \theta) \in \mathbb{T}^3 \end{aligned} \qquad [7]$$

are conjugate symplectic coordinates and if $\phi_{\rm Del}$ is the corresponding symplectic map, then $\mathcal{H}_{\rm Kep} \circ \phi_{\rm Del} = -(\mu^3 M^2)/(2L^2)$.

Note that the Delaunay variables become singular when C is vertical (the node is no more defined) and in the circular limit (the perihelion is not unique). In these cases different variables have to be used.

5. Let $(X^{(i)}, x^{(i)}) = \phi_{\rm Del}((L_i, G_i, \Theta_i), (\ell_i, g_i, \theta_i))$. Then $\mathcal{H}_{\rm plt}$ expressed in the Delaunay variables $\{(L_i, G_i, \Theta_i), (\ell_i, g_i, \theta_i): 1 \le i \le n\}$ becomes

$$\mathcal{H}_{\rm Del} = \mathcal{H}^{(0)}_{\rm Del} + \varepsilon \mathcal{H}^{(1)}_{\rm Del}, \quad \mathcal{H}^{(0)}_{\rm Del} := -\sum_{i=1}^{n} \frac{\mu_i^3 M_i^2}{2L_i^2} \qquad [8]$$

Note that the number of action variables on which the integrable Hamiltonian $\mathcal{H}^{(0)}_{\rm Del}$ depends is strictly less than the number of degrees of freedom. This "proper degeneracy," as we shall see in next sections, brings in an essential difficulty one has to face in the perturbative approach to the many-body problem. In fact, this feature of the many-body problem is common to several other problems of celestial mechanics.

Maximal KAM Tori

Kolmogorov's Theorem and the RPC3BP (1954)

Kolmogorov's invariant tori theorem deals with the persistence, in nearly integrable Hamiltonian systems, of Lagrangian (maximal) tori, which, in general, foliate the integrable limit. Kolmogorov (1954) stated his theorem and gave a precise outline of the proof. Let us briefly recall this milestone of the modern theory of dynamical systems.

Let $\mathcal{M} := B^d \times \mathbb{T}^d$ (B^d being a d-dimensional ball in $\mathbb{R}^d$ centered at the origin) be endowed with the standard symplectic form $dy \wedge dx := \sum dy_i \wedge dx_i$ ($y \in B^d$, $x \in \mathbb{T}^d$). A Hamiltonian function N on $\mathcal{M}$ having a Lagrangian invariant d-torus of energy E on which the N-flow is conjugated to the linear dense translation $x \to x + \omega t$, $\omega \in \mathbb{R}^d \setminus \mathbb{Q}^d$ can be put in the form

$$\begin{aligned} &N := E + \omega \cdot y + Q(y, x) \\ &\partial_y^\alpha Q(0, x) = 0, \quad \forall \alpha \in \mathbb{N}^d, \quad |\alpha| \le 1 \end{aligned} \qquad [9]$$

(as usual, $|\alpha| = \alpha_1 + \cdots + \alpha_d$, $\omega \cdot y := \sum_{i=1}^d \omega_i y_i$, and $\partial_y^\alpha = \partial_{y_1}^{\alpha_1} \cdots \partial_{y_d}^{\alpha_d}$); in such a case, the Hamiltonian N is said to be in Kolmogorov normal form. The vector ω is called the "frequency vector" of the invariant torus $\{y = 0\} \times \mathbb{T}^d$. The Hamiltonian N is said to be nondegenerate if

$$\det \langle \partial_y^2 Q(0, \cdot) \rangle \ne 0 \qquad [10]$$

where the brackets denote average over $\mathbb{T}^d$ and ∂_y^2 the Hessian with respect to the y-variables.

We recall that a vector $\omega \in \mathbb{R}^d$ is said to be "Diophantine" if there exist $\kappa > 0$ and $\tau \ge d - 1$ such that

$$|\omega \cdot k| \ge \frac{\kappa}{|k|^\tau}, \quad \forall k \in \mathbb{Z}^d \setminus \{0\} \qquad [11]$$

The set $\mathcal{D}^d$ of all Diophantine vectors in $\mathbb{R}^d$ is a set of full Lebesgue measure. We also recall that Hamiltonian trajectory is called quasiperiodic with (rationally independent) frequency $\omega \in \mathbb{R}^d$ if it is conjugate to the linear translation $\theta \in \mathbb{T}^d \to \theta + \omega t \in \mathbb{T}^d$.

Theorem (Kolmogorov 1954) *Consider a one-parameter family of real-analytic Hamiltonian functions $H_\varepsilon := N + \varepsilon P$ where N is in Kolmogorov normal form (as in* eqn [9]*) and $\varepsilon \in \mathbb{R}$. Assume that ω is Diophantine and that N is nondegenerate. Then, there exists $\varepsilon_0 > 0$ and for any $|\varepsilon| \le \varepsilon_0$, a real-analytic symplectic transformation $\phi_\varepsilon : \mathcal{M} \to \mathcal{M}$ putting H_ε in Kolmogorov normal form, $H_\varepsilon \circ \phi_\varepsilon = N_\varepsilon$, with $N_\varepsilon := E_\varepsilon + \omega \cdot y' + Q_\varepsilon(y', x')$. Furthermore, $|E_\varepsilon - E|$, $\|\phi_\varepsilon - {\rm id}\|_{C^2}$, and $\|Q_\varepsilon - Q\|_{C^2}$ are small with ε.*

In other words, the Lagrangian unperturbed torus $\mathcal{T}_0 := \{y = 0\} \times \mathbb{T}^d$ persists under small perturbation and is smoothly deformed into the H_ε-invariant torus $\mathcal{T}_\varepsilon := \phi_\varepsilon(\{y' = 0\} \times \mathbb{T}^d)$; the dynamics on such torus, for all $|\varepsilon| \leq \varepsilon_0$, consists of dense quasiperiodic trajectories. Note that the H_ε-flow on $\mathcal{T}_\varepsilon$ is analytically conjugated by ϕ_ε to the translation $x' \to x' + \omega t$ with the same frequency vector of N, while the energy of $\mathcal{T}_\varepsilon$, namely E_ε, is in general different from the energy E of $\mathcal{T}_0$.

Kolmogorov's proof is based on an iterative (Newton) scheme. The map ϕ_ε is obtained as $\lim_{k\to\infty} \phi^{(1)} \circ \cdots \circ \phi^{(k)}$, where the $\phi^{(j)}$'s are (ε-dependent) symplectic transformations of $\mathcal{M}$ successively closer to the identity. It is enough to describe the construction of $\phi^{(1)}$; $\phi^{(2)}$ is then obtained by replacing H_ε with $H_\varepsilon \circ \phi^{(1)}$, and so on. The map $\phi^{(1)}$ is ε-close to the identity and it is generated by $g(y', x) := y' \cdot x + \varepsilon(b \cdot x + s(x) + y' \cdot a(x))$, where s and a are (resp. scalar- and vector-valued) real-analytic functions on $\mathbb{T}^d$ with zero average and $b \in \mathbb{R}^d$; this means that the symplectic map $\phi^{(1)} : (y', x') \to (y, x)$ is implicitly given by the relations $y = \partial_x g$ and $x' = \partial_{y'} g$. It is easy to see that there exists a unique g of the above form such that for a suitable $\varepsilon_0 > 0$,

$$H_\varepsilon \circ \phi^{(1)} = E_1 + \omega \cdot y' + Q_1(y', x') + \varepsilon^2 P_1 \quad \forall\ |\varepsilon| \leq \varepsilon_0 \qquad [12]$$

with $\partial_y^\alpha Q_1(0, x') = 0$, for any $\alpha \in \mathbb{N}^d$ and $|\alpha| \leq 1$; here, E_1, Q_1, and P_1 depend on ε and, for a suitable $c_1 > 0$ and for $|\varepsilon| \leq \varepsilon_0$, $|E - E_1| \leq c_1|\varepsilon|$, $\|Q - Q_1\|_{C^2} \leq c_1|\varepsilon|$, and $\|P_1\|_{C^2} \leq c_1$.

Notice that the symplectic transformation $\phi^{(1)}$ is actually the composition of two "elementary" transformations: $\phi^{(1)} = \phi_1^{(1)} \circ \phi_2^{(1)}$ where $\phi_2^{(1)}: (y', x') \to (\eta, \xi)$ is the symplectic lift of the $\mathbb{T}^d$-diffeomorphism given by $x = \xi + \varepsilon a(\xi)$ (i.e., $\phi_2^{(1)}$ is the symplectic map generated by $y' \cdot \xi + \varepsilon y' \cdot a(\xi)$), while $\phi_1^{(1)} : (\eta, \xi) \to (y, x)$ is the angle-dependent action translation generated by $\eta \cdot x + \varepsilon(b \cdot x + s(x))$; $\phi_2^{(1)}$ acts in the "angle direction" and straightens out the flow up to order $O(\varepsilon^2)$, while $\phi_1^{(1)}$ acts in the "action direction" and is needed to keep the frequency of the torus fixed.

Since $H_\varepsilon \circ \phi_1 =: N_1 + \varepsilon^2 P_1$ is again a perturbation of a nondegenerate Kolmogorov normal form (with same frequency vector ω), one can repeat the construction by obtaining a new Hamiltonian of the form $N_2 + \varepsilon^4 P_2$. Iterating, after k steps, one gets a Hamiltonian $N_k + \varepsilon^{2^k} P_k$. Carrying out the (straightforward but lengthy) estimates, one can check that $\|P_k\|_{C^2} \leq c_k \leq c^{2^k}$, for a suitable constant $c > 1$ independent of k (the fast growth of the constant c_k is due to the presence of the small divisors appearing in the explicit construction of the symplectic transformations $\phi^{(j)}$). Thus, it is clear that taking ε_0 small enough the iterative procedure converges (superexponentially fast) yielding the thesis of the above theorem.

6. While the statement of the invariant tori theorem and the outline of the proof are very clearly explained in Kolmogorov (1954), Kolmogorov did not fill out the details nor gave any estimates. Some years later, Arnol'd (1963a) published a detailed proof, which, however, did not follow Kolmogorov's idea. In the same year, J K Moser published his invariant curve theorem (for area-preserving twist diffeomorphisms of the annulus) in smooth setting. The bulk of techniques and theorems stemmed out from these works is normally referred to as KAM theory; for reviews, see Arnol'd (1988) or Bost (1984–85). A very complete version of the "KAM theorem" both in the real-analytic and in the smooth case (with optimal smoothness assumptions) is given in Salamon (2004); the proof of the real-analytic part is based on Kolmogorov's scheme. The KAM theory of M Herman, used in his approach to the planetary problem, is based on the abstract functional theoretical approach of R Hamilton (which, in turn, is a development of Nash–Moser implicit function theorem; see Bost (1984–85) for references); it is interesting, however, to note that the heart of Herman's KAM method is based on the above-mentioned Kolmogorov's transformation $\phi^{(1)}$ (compare Féjoz (2002)).
7. In the nearly integrable case, one considers a one-parameter family of Hamiltonians $H_0(I) + \varepsilon H_1(I, x)$ with $(I, x) \in \mathcal{M} := U \times \mathbb{T}^d$ standard symplectic action-angle variables, U being an open subset of $\mathbb{R}^d$. When $\varepsilon = 0$, the phase space $\mathcal{M}$ is foliated by H_0-invariant tori $\{I_0\} \times \mathbb{T}^d$, on which the flow is given by $x \to x + \partial_y H_0(I_0)t$. If I_0 is such that $\omega := \partial_y H_0(I_0)$ is Diophantine and if $\det \partial_y^2 H_0(I_0) \neq 0$, then from Kolmogorov's theorem it follows that the torus $\{I_0\} \times \mathbb{T}^d$ persists under perturbation. In fact, introduce the symplectic variables (y, x) with $y = I - I_0$ and let $N(y) := H_0(I_0 + y)$, which by Taylor's formula can be written as $H_0(I_0) + \omega \cdot y + Q(y)$ with $Q(y)$ quadratic in y and $\partial_y^2 Q(0) = \partial_y^2 H_0(I_0)$ invertible. One can then apply Kolmogorov's theorem with $P_1(y, x) := H_1(I_0 + y, x)$.

   Notice that Kolmogorov's nondegeneracy condition $\det \partial_y^2 H_0(I_0) \neq 0$ simply means that the frequency map

$$I \in B^d \subset U \to \omega(I) := \partial_y H_0(I) \qquad [13]$$

is a local diffeomorphism (B^d being a ball around I_0).

8. The symplectic structure implies that if n denotes the number of degrees of freedom (i.e., half of the dimension of the phase space) and d is the number of independent frequencies of a quasi-periodic motion, then $d \leq n$; if $d = n$, the quasi-periodic motion is called maximal. Kolmogorov's theorem gives sufficient conditions in order to get maximal quasiperiodic solutions. In fact, Kolmogorov's nondegeneracy condition is an open condition and the set of Diophantine vectors is a set of full Lebesgue measure. Thus, in general, Kolmogorov's theorem yields a positive invariant measure set spanned by maximal quasiperiodic trajectories.

As mentioned above, the planetary many-body models are properly degenerate and violate Kolmogorov's nondegeneracy conditions and, hence, Kolmogorov's theorem – clearly motivated by celestial mechanics – cannot be applied.

There is, however, an important case to which a slight variation of Kolmogorov's theorem can be applied (Kolmogorov did not mention this in 1954). The case referred to here is the simplest nontrivial three-body problem, namely, the restricted, planar, and circular three-body problem (RPC3BP for short). This model, largely investigated by Poincaré, deals with an asteroid of "zero mass" moving on the plane containing the trajectory of two unperturbed major bodies (say, Sun and Jupiter) revolving on a Keplerian circle. The mathematical model for the restricted three-body problem is obtained by taking $n = 2$ and setting $m_2 = 0$ in eqn [1]: the equations for the two major bodies $(i = 0, 1)$ decouple from the equation for the asteroid $(i = 2)$ and form an integrable two-body system; the problem then consists in studying the evolution of the asteroid $u^{(2)}(t)$ in the given gravitational field of the primaries. In the circular and planar cases, the motion of the two primaries is assumed to be circular and the motion of the asteroid is assumed to take place on the plane containing the motion of the two primaries; in fact (to avoid collisions), one considers either inner or outer (with respect to the circle described by the relative motion of the primaries) asteroid motions. To describe the Hamiltonian $\mathcal{H}_{\rm rcp}$ governing the motion of the RCP3BP problem, introduce planar Delaunay variables $((L, G), (\ell, \hat{g}))$ for the asteroid (better, for the reduced heliocentric Sun–asteroid system). Such variables, which are closely related to the above (spatial) Delaunay variables, have the following physical interpretation: G is proportional to the absolute value of the angular momentum of the asteroid, L is proportional to the square root of the semimajor axis of the instantaneous Sun–asteroid ellipse, ℓ is the mean anomaly of the asteroid, while $\hat{g}$ the argument of the perihelion. Then, in suitably normalized units, the Hamiltonian governing the RPC3BP is given by

$$\mathcal{H}_{\rm rcp}(L, G, \ell, g; \varepsilon) := -\frac{1}{2L^2} - G + \varepsilon \mathcal{H}_1(L, G, \ell, g; \varepsilon) \quad [14]$$

where $g := \hat{g} - \tau, \tau \in \mathbb{T}$ being the longitude of Jupiter; the variables $((L, G), (\ell, g))$ are symplectic coordinates (with respect to the standard symplectic form); the normalizations have been chosen so that the relative motion of the primary bodies is 2π periodic and their distance is 1; the parameter ε is (essentially) the ratio between the masses of the primaries; the perturbation $\mathcal{H}_1$ is the function $x^{(2)} \cdot x^{(1)} - 1/|x^{(2)} - x^{(1)}|$ expressed in the above variables, $x^{(2)}$ being the heliocentric coordinate of the asteroid and $x^{(1)}$ that of the planet (Jupiter): such a function is real-analytic on $\{0 < G < L\} \times \mathbb{T}^2$ and for small ε (for complete details, see, e.g., Celletti and Chierchia (2003)).

The integrable limit

$$\mathcal{H}^{(0)}_{\rm rcp} := \mathcal{H}_{\rm rcp}|_{\varepsilon = 0} = -1/(2L^2) - G$$

has vanishing Hessian and, hence, violates Kolmogorov's nondegeneracy condition (as described in item (7) above). However, there is another nondegeneracy condition which leads to a simple variation of Kolmogorov's theorem, as explained briefly below.

Kolmogorov's nondegeneracy condition $\det_y^2 H_0(I_0) \neq 0$ allows one to fix d-parameters, namely, the d-components of the (Diophantine) frequency vector $\omega = \partial_y H_0(I_0)$. Instead of fixing such parameters, one may fix the energy $E = H_0(I_0)$ together with the direction $\{s\omega : s \in \mathbb{R}\}$ of the frequency vector: for example, in a neighborhood where $\omega_d \neq 0$, one can fix E and ω_i/ω_d for $1 \leq i \leq d - 1$. Notice also that if ω is Diophantine, then so is $s\omega$ for any $s \neq 0$ (with same τ and rescaled κ). Now, it is easy to check that the map $I \in H_0^{-1}(E) \to (\omega_1/\omega_d, \ldots, \omega_{d-1}/\omega_d)$ is (at fixed energy E) a local diffeomorphism if and only if the $(d+1) \times (d+1)$ matrix

$$\begin{pmatrix} \partial_y^2 H_0 & \partial_y H_0 \\ \partial_y H_0 & 0 \end{pmatrix}$$

evaluated at I_0 is invertible (here the vector $\partial_y H_0$ in the upper right corner has to be interpreted as a column while the vector $\partial_y H_0$ in the lower left corner has to be interpreted as a row). Such

"iso-energetic nondegeneracy" condition, rephrased in terms of Kolmogorov's normal forms, becomes

$$\det\begin{pmatrix} \langle \partial_y^2 Q(0,\cdot)\rangle & \omega \\ \omega & 0 \end{pmatrix} \neq 0 \qquad [15]$$

Kolmogorov's theorem can be easily adapted to the fixed energy case. Assuming that ω is Diophantine and that N is isoenergetically nondegenerate, the same conclusion as in Kolmogorov's theorem holds with $N_\varepsilon := E + \omega_\varepsilon \cdot y' + Q_\varepsilon(y', x')$, where $\omega_\varepsilon = \alpha_\varepsilon \omega$ and $|\alpha_\varepsilon - 1|$ is small with ε.

In the RCP3BP case, the isoenergetic nondegeneracy is met, since

$$\det\begin{pmatrix} \partial^2_{(L,G)}\mathcal{H}^{(0)}_{\rm rcp} & \partial_{(L,G)}\mathcal{H}^{(0)}_{\rm rcp} \\ \partial_{(L,G)}\mathcal{H}^{(0)}_{\rm rcp} & 0 \end{pmatrix} = \frac{3}{L^4}$$

Therefore, one can conclude that on each negative energy level, the RCP3BP admits a positive measure set of phase points, whose time evolution lies on two-dimensional invariant tori (on which the flow is analytically conjugate to linear translation by a Diophantine vector), provided the mass ratio of the primary bodies is small enough; such persistent tori are a slight deformation of the unperturbed "Keplerian" tori corresponding to the asteroid and the Sun revolving on a Keplerian ellipse on the plane where the Sun and the major planet describe a circular orbit.

In fact, one can say more. The phase space for the RCP3BP is four dimensional, the energy levels are three dimensional, and Kolmogorov's invariant tori are two dimensional. Thus, a Kolmogorov torus separates the energy level, on which it lies, into two invariant components, and two Kolmogorov's tori form the boundary of a compact invariant region so that any motion starting in such region will never leave it. Thus, the RCP3BP is "totally stable": in a neighborhood of any phase point of negative energy, if the mass ratio of the primary bodies is small enough, the asteroid stays forever on a nearly Keplerian ellipse with nearly fixed orbital elements L and G.

Arnol'd's Theorem

Consider again the planetary $(1+n)$-body problem governed by the Hamiltonian $\mathcal{H}_{\rm plt}$ in eqn [5]. In the integrable approximation, governed by the Hamiltonian $\mathcal{H}^{(0)}_{\rm plt}$, the n planets describe Keplerian ellipses focused on the Sun. Arnol'd (1963b) has stated the following theorem.

Theorem (Arnol'd 1963b) *Let $\varepsilon > 0$ be small enough. Then, there exists a bounded, $\mathcal{H}_{\rm plt}$-invariant set $\mathcal{F}(\varepsilon) \subset \mathcal{M}$ of positive Lebesgue measure corresponding to planetary motions with bounded relative distances; $\mathcal{F}(0)$ corresponds to Keplerian ellipses with small eccentricities and small relative inclinations.*

This theorem represents a major achievement in celestial mechanics solving more than tri-ĉentennial mathematical problem. Arnol'd (1963b) gave a complete proof of this result only in the planar three-body case and gave some indications of how to extend his approach to the general situation. However, to give a full proof of Arnol'd's theorem in the general case turned out to be more than a technical problem and new ideas were needed: the complete proof (due, essentially, to M Herman) has been given only in 2004.

In the following subsections, we briefly review the history and the ideas related to the proof of Arnol'd's theorem. As for credits: the proof of Arnol'd's theorem in the planar 3BP case is due to Arnol'd himself (Arnol'd 1963b); the spatial 3BP case is due to Laskar and Robutel (1995) and Robutel (1995); the general case is due to Herman (1998) and Féjoz (2004). The exposition we have given does not always follow the original references.

The planar three-body problem Recall the Hamiltonian $\mathcal{H}_{\rm pln}$ of the planar $(1+n)$-body problem given in item (3) of the section "The planetary $(1+n)$-body problem." A convenient set of symplectic variables for nearly circular motions are the "planar Poincaré variables." To describe such variables, consider a single, planar two-body system with Hamiltonian

$$\frac{|X|^2}{2\mu} - \frac{\mu M}{|x|}, \quad X \in \mathbb{R}^2, \quad 0 \neq x \in \mathbb{R}^2 \quad \text{(with respect to } dX \wedge dx\text{)} \qquad [16]$$

and introduce – as done before formula [14] for $\mathcal{H}^{(0)}_{\rm rcp}$ – planar Delaunay variables $((L,G),(\ell,g))$ (here, $g = \hat{g} =$ argument of the perihelion). To remove the singularity of the Delaunay variables near zero eccentricities, Poincaré introduced variables $((\Lambda,\eta),(\lambda,\xi))$ defined by the following formulas:

$$\begin{aligned} &\Lambda = L, \quad H = L - G \\ &\lambda = \ell + g, \quad h = -g \\ &\sqrt{2H}\cos h = \eta \\ &\sqrt{2H}\sin h = \xi \end{aligned} \qquad [17]$$

As Poincaré showed, such variables are symplectic and analytic in a neighborhood of $(0,\infty)\times\mathbb{T}\times\{0,0\}$; notice that the symplectic map $((\Lambda,\eta),(\lambda,\xi)) \to (X,x)$ depends on the parameters μ, M, and ε. In Poincaré variables, the two-body Hamiltonian in eqn [16]

becomes $-\kappa/(2\Lambda^2)$, with $\kappa := (\mu/m_0)^3/M$. Now, re-insert the index i, let $\phi_i : ((\Lambda_i, \eta_i), (\lambda_i, \xi_i)) \to (X^{(i)}, x^{(i)})$ and $\phi(\Lambda, \eta, \lambda, \xi) = (\phi_1(\Lambda_1, \eta_1, \lambda_1, \xi_1), \ldots, \phi_n(\Lambda_n, \eta_n, \lambda_n, \xi_n))$. Then, the Hamiltonian for the planar $(1+n)$-body problem takes the form

$$\begin{aligned} \mathcal{H}_{\text{pln}} \circ \phi &= \mathcal{H}_0(\Lambda) + \varepsilon \mathcal{H}_1(\Lambda, \lambda, \eta, \xi) \\ \mathcal{H}_0 &:= -\frac{1}{2}\sum_{i=1}^{n} \frac{\kappa_i}{\Lambda_i^2}, \quad \kappa_i := \left(\frac{\mu_i}{m_0}\right)^3 \frac{1}{M_i} \\ \mathcal{H}_1 &:= \mathcal{H}_1^{\text{compl}} + \mathcal{H}_1^{\text{princ}} \end{aligned} \tag{18}$$

where the so-called "complementary part" $\mathcal{H}_1^{\text{compl}}$ and the "principal part" $\mathcal{H}_1^{\text{princ}}$ of the perturbation are, respectively, the functions

$$\sum_{1 \le i < j \le n} X^{(i)} \cdot X^{(j)} \quad \text{and} \quad \sum_{1 \le i < j \le n} \frac{\mu_i \mu_j}{m_0^2} \frac{1}{|x^{(i)} - x^{(j)}|} \tag{19}$$

expressed in Poincaré variables.

The scheme of proof of Arnol'd's theorem in the planar, three-body case (one star, $n=2$ planets) is as follows. The Hamiltonian is given by eqn [13] with $n=2$; the phase space is eight dimensional (four degrees of freedom). This system, as mentioned several times, is properly degenerate and Kolmogorov's theorem cannot be applied directly; furthermore, a full (four-dimensional) set of action variables needs to be identified.

A first observation is that, in the planetary model, there are "fast variables" (the λ_i's describing the revolutions of the planets) and "secular variables" (the η_i's and ξ_i's describing the variations of position and shape of the instantaneuous Keplerian ellipses). By averaging theory (see, e.g., Arnol'd (1998)), one can "neglect," in nonresonant regions, the fast-angle dependence up to high order in ε obtaining an effective Hamiltonian, which, up to $O(\varepsilon^2)$, is given by the "secular" Hamiltonian

$$\begin{aligned} \mathcal{H}_{\text{sec}} &:= \mathcal{H}_0(\Lambda) + \varepsilon \bar{\mathcal{H}}_1(\Lambda, \eta, \xi) \\ \bar{\mathcal{H}}_1(\Lambda, \eta, \xi) &:= \int \mathcal{H}_1 \frac{\mathrm{d}\lambda}{(2\pi)^2} \end{aligned} \tag{20}$$

"Nonresonant region" means, here, an open Λ-set where $\partial_\Lambda \mathcal{H}_0 \cdot k \neq 0$ for $k \in \mathbb{Z}^2, |k_1| + |k_2| \le K$ and for a suitable $K \ge 1$.

In order to analyze the secular Hamiltonian, we shall beriefly consider $\bar{\mathcal{H}}_1$ as a function of the symplectic variables η and ξ, regarding the "slow actions" Λ_i as parameters.

For symmetry reasons, $\bar{\mathcal{H}}_1$ is even in (η, ξ) and the point $(\eta, \xi) = (0, 0)$ is an elliptic equilibrium for $\bar{\mathcal{H}}_1$: the eigenvalues of the matrix $S\partial^2_{(\eta,\xi)}\bar{\mathcal{H}}_1(\Lambda, 0, 0)$, S being the standard symplectic matrix, are purely imaginary numbers $\{\pm \mathrm{i}\Omega_1, \pm \mathrm{i}\Omega_2\}$. The real numbers $\{\Omega_i\}$ are symplectic invariants of the secular Hamiltonian and are usually called first (or linear) Birkhoff invariants. In a neighborhood of an elliptic equilibrium, one can use Birkhoff's normal form theory (see, e.g., Siegel (1971)): if the linear invariants (Ω_1, Ω_2) are nonresonant up to order r (i.e., if $\Omega \cdot k := \Omega_1 k_1 + \Omega_2 k_2 \neq 0$ for any $k \in \mathbb{Z}^2$ such that $|k_1| + |k_2| \le r$), then one can find a symplectic transformation ϕ_{Bir} so that

$$\bar{\mathcal{H}}_1 \circ \phi_{\text{Bir}} = F(J_1, J_2; \Lambda) + o_r, \quad J_j = \frac{\eta_j^2 + \xi_j^2}{2} \tag{21}$$

where F is a polynomial of degree $[r/2]$ of the form $\Omega_1 J_1 + \Omega_2 J_2 + (1/2)\mathcal{M}J \cdot J + \cdots$, $\mathcal{M} = \mathcal{M}(\Lambda)$ being a (2×2) matrix (and $o_r/|J|^{r/2} \to 0$ as $|J| \to 0$). Arnol'd, using computations performed by Le Verrier, checked the nonresonance condition up to order $r=6$ in the asymptotic regime $a_1/a_2 \to 0$ (where a_i denote the semimajor axes of approximate Keplerian ellipses of the two planets); these computations represent one of the most delicate parts of the paper.

Thus, combining averaging theory and Birkhoff normal form theory, one can construct a symplectic change of variables defined on an open subset of the phase space (avoiding some linear resonances) $(\Lambda, \lambda, \eta, \xi) \to (\Lambda', \lambda', J, \varphi)$, where $\eta_j + \mathrm{i}\xi_j = \sqrt{2J_j}\exp(\mathrm{i}\varphi_j)$, casting the three-body Hamiltonian into the form

$$\begin{aligned} &\mathcal{H}_0(\Lambda') + \varepsilon\left(\Omega(\Lambda') \cdot J + \tfrac{1}{2}\mathcal{M}(\Lambda')J \cdot J\right) \\ &\quad + \varepsilon^2 \mathcal{F}_1(\Lambda', J) + \varepsilon^p \mathcal{F}_2(\Lambda', \lambda', J, \varphi) \\ &\quad := \tilde{\mathcal{H}}_0(\Lambda', J; \varepsilon) + \varepsilon^p \mathcal{F}_2(\Lambda', \lambda', J, \varphi) \end{aligned} \tag{22}$$

for a suitable prefixed order $p \ge 3$; notice that the nonresonance condition needed to apply averaging theory is not particularly hard to check since it involves the unperturbed and completely explicit Kepler Hamiltonian $\mathcal{H}_0$. The idea is now to consider $\varepsilon^p \mathcal{F}_2$ as a perturbation of the completely integrable Hamiltonian $\tilde{\mathcal{H}}_0$ and to apply Kolmogorov's theorem. Finally, one can check the Kolmogorov's nondegenearcy condition, which since

$$\det \partial^2_{(\Lambda', J)} \tilde{\mathcal{H}}_0(\Lambda', J'; \varepsilon) = \varepsilon^2\left((\det \mathcal{H}_0'') \det \mathcal{M} + O(\varepsilon)\right)$$

amounts to check the invertibility of the matrix $\mathcal{M}$. Such a condition is also checked in Arnol'd (1963b) with the aid of Le Verrier's tables and in the asymptotic regime $a_1/a_2 \to 0$.

The spatial three-body problem In order to extend the previous argument to the spatial case, Arnol'd suggested connecting the planar and spatial case through a limiting procedure. Such strategy presents

analytical problems (the symplectic variables for the spatial case become singular in the planar limit), which have not been overcome. However, the particular structure of the three-body case allows one to derive a four-degree-of-freedom Hamiltonian, to which the proof of the planar case can be easily adapted. The procedure described below is based on the classical Jacobi's reduction of the nodes.

First, we inroduce a convenient set of symplectic variables. Let, for $i=1,2,((L_i,G_i,\Theta_i),(\ell_i,g_i,\theta_i))$ denote the Delaunay variables introduced in items (5) and (6) above: these are the Delaunay variables associated to the two-body system, Sun–ith planet. Then, as Poincaré showed, the variables $((\Lambda_i^*,\lambda_i^*),(\eta_i^*,\xi_i^*),(\Theta_i,\theta_i))$, where

$$\begin{aligned}\Lambda_i^* &= L_i\\ \lambda_i^* &= \ell_i+g_i\\ \eta_i^* &= \sqrt{2(L_i-G_i)}\cos g_i\\ \xi_i^* &= -\sqrt{2(L_i-G_i)}\sin g_i\end{aligned} \qquad [23]$$

are symplectic and analytic near circular, non-coplanar motions; for a detailed discussion of these and other sets of interesting classical variables, see, for example, Biasco *et al.* (2003) and references therein; the asterisk is introduced to avoid confusion with a closely related but different set of Poincaré variables (see below). Let us denote by

$$\mathcal{H}_{3\text{bp}} := \mathcal{H}^{(0)}(\Lambda^*) + \varepsilon\mathcal{H}^{(1)}(\Lambda^*,\lambda^*,\eta^*,\xi^*,\Theta,\theta)$$

the Hamiltonian equation [8] (with $n=2$) expressed in terms of the symplectic variables $((\Lambda^*,\lambda^*),(\eta^*,\xi^*),(\Theta,\theta)),\Lambda^*=(\Lambda_1^*,\Lambda_2^*)$, etc. Recalling the physical meaning of the Delaunay variables, one realizes that $\Theta_1+\Theta_2$ is the vertical component, $C_3=C\cdot k_3$, of the total argument $C=C^{(1)}+C^{(2)}$, where $C^{(i)}$ denotes the angular momentum of the ith planet with respect to the origin of an inertial heliocentric frame $\{k_1,k_2,k_3\}$. This suggests that the symplectic variables can be introduced:

$$(\Lambda^*,\lambda^*,\eta^*,\xi^*,\Psi,\psi) = \phi(\Lambda^*,\lambda^*,\eta^*,\xi^*,\Theta,\theta)$$

with $(\Psi_1,\Psi_2,\psi_1,\psi_2):=(\Theta_1,\Theta_1+\Theta_2,\theta_1-\theta_2,\theta_2)$.

Let

$$\mathcal{H}_{3\text{bp}}^* := \mathcal{H}_{3\text{bp}}\circ\phi^{-1}$$

denote the Hamiltonian of the spatial three-body problem in these symplectic variables. Since the Poisson bracket of $\Psi_2=\Theta_1+\Theta_2$ and $\mathcal{H}_{3\text{bp}}^*$ vanishes (C_3 being an integral for the $\mathcal{H}_{3\text{bp}}$-flow), the conjugate angle ψ_2 is cyclic for $\mathcal{H}_{3\text{bp}}^*$, that is,

$$\mathcal{H}_{3\text{bp}}^* = \mathcal{H}_{3\text{bp}}^*(\Lambda^*,\lambda^*,\eta^*,\xi^*,\Psi_1,\Psi_2,\psi_1)$$

Now (because the total angular momentum C is preserved), one may restrict attention to the ten-dimensional invariant (and symplectic) submanifold $\mathcal{M}_{\text{ver}}$ defined by fixing the total angular momentum to be vertical. Such submanifold is easily described in terms of Delaunay variables; in fact, $C\cdot k_1=0=C\cdot k_2$ is equivalent to

$$\theta_1-\theta_2=\pi \quad\text{and}\quad G_1^2-\Theta_1^2=G_2^2-\Theta_2^2 \qquad [24]$$

Thus, $\mathcal{M}_{\text{ver}}^* := \phi(\mathcal{M}_{\text{ver}})$ is given by

$$\mathcal{M}_{\text{ver}}^* = \left\{\psi_1=\pi,\ \Psi_1=\widehat{\Psi}_1(\Lambda^*,\eta^*,\xi^*;\Psi_2)\right\}$$

with

$$\begin{aligned}\widehat{\Psi}_1 &:= \frac{\Psi_2}{2}+\frac{(\Lambda_1^*-H_1^*)^2-(\Lambda_2^*-H_2^*)^2}{2\Psi_2}\\ H_i^* &:= \frac{\eta_i^{*2}+\xi_i^{*2}}{2}\end{aligned}$$

Since $\mathcal{M}_{\text{ver}}^*$ is invariant for the flow ϕ_*^t of $\mathcal{H}_{3\text{bp}}^*$, $\psi_1(t)\equiv\pi$ and $\dot{\psi}_1\equiv 0$ for motions starting on $\mathcal{M}_{\text{ver}}^*$, which implies that $(\partial_{\Psi_1}\mathcal{H}_{3\text{bp}}^*)|_{\mathcal{M}_{\text{ver}}^*}=0$. This fact allows one to introduce, for fixed values of the vertical angular momentum $\Psi_2=c\neq 0$, the following reduced Hamiltonian

$$\begin{aligned}&\mathcal{H}_{\text{red}}^c(\Lambda^*,\lambda^*,\eta^*,\xi^*)\\ &\quad := \mathcal{H}_{3\text{bp}}^*(\Lambda^*,\lambda^*,\eta^*,\xi^*,\ \widehat{\Psi}_1(\Lambda^*,\eta^*,\xi^*;c),c,\pi)\end{aligned}$$

on the eight-dimensional phase space $\mathcal{M}_{\text{red}} := \{\Lambda_i^*>0,\ \lambda\in\mathbb{T}^2,(\eta^*,\xi^*)\in B^4\}$ endowed with the standard symplectic form $d\Lambda^*\wedge d\lambda^*+d\eta^*\wedge d\xi^*$ (B^4 being a ball around the origin in $\mathbb{R}^4$). In fact, the (standard) Hamilton's equations for $\mathcal{H}_{\text{red}}^c$ are immediately recognized to be a subsystem of the full (standard) Hamilton's equations for $\mathcal{H}_{3\text{bp}}$ when the initial data are restricted on $\mathcal{M}_{\text{ver}}^*$ and the constant value of Ψ_2 is chosen to be c. More precisely, if the Hamiltonian flow of $\mathcal{H}_{\text{red}}^c$ on $\mathcal{M}_{\text{red}}$ is denoted by ϕ_c^t, then

$$\begin{aligned}&\phi_*^t\left(z^*,\widehat{\Psi}_1(\Lambda^*,\eta^*,\xi^*;c),c,\pi,\psi_2\right)\\ &\quad=\left(\phi_c^t(z^*),\widehat{\Psi}_1(t),c,\pi,\psi_2(t)\right)\end{aligned} \qquad [25]$$

where we have used the shorthand notations: $z^*=(\Lambda^*,\lambda^*,\eta^*,\xi^*)\in\mathcal{M}_{\text{red}}$; $\widehat{\Psi}_1(t)=\widehat{\Psi}_1\circ\phi_c^t(z^*)$; $\psi_2(t)=\psi_2+\int_0^t\partial_{\Psi_2}\mathcal{H}_{3\text{bp}}^*(\phi_c^s(z^*),\widehat{\Psi}_1(s),c,\pi)ds$. At this point, the scheme used for the planar case may be easily adapted to the present situation. The nondegeneracy conditions have been checked in Robutel (1995) where indications, based on a computer program, have been given for the validity of the theorem in a wider set of initial data.

Notice that the dimension of the reduced phase space of the spatial case is 8, which is also the dimension of the phase space of the planar case.

Therefore, also the Lagrangian tori obtained with this procedure have the same dimension of the tori obtained in the planar case (i.e., four).

The general case Consider the general case following the strategy of M Herman as presented by Féjoz (2004), to which the reader is referred for complete proofs and further references.

The symplectic variables used in Féjoz (2004), to cope with the spatial planetary $(1+n)$-body problem (Sun and n planets), are closely related to the variables defined in eqn [23]. For $1 \le i \le n$, let $((L_i, G_i, \Theta_i), (\ell_i, g_i, \theta_i))$ denote the Delaunay variables associated with the two-body system, Sun–ith planet. Then (as shown by Poincaré) the variables $((\Lambda_i, \lambda_i), (\eta_i, \xi_i), (p_i, q_i))$, where $\Lambda_i = L_i$, $\lambda_i = \ell_i + g_i + \theta_i$, and

$$\begin{aligned} \eta_i &= \sqrt{2(L_i - G_i)}\cos(g_i + \theta_i) \\ \xi_i &= -\sqrt{2(L_i - G_i)}\sin(g_i + \theta_i) \\ p_i &= \sqrt{2(G_i - \Theta_i)}\cos\theta_i \\ q_i &= -\sqrt{2(G_i - \Theta_i)}\sin\theta_i \end{aligned} \qquad [26]$$

are symplectic and analytic near circular, noncoplanar motions (see, e.g., Biasco *et al.* (2003)). Let

$$\mathcal{H}_{\mathrm{nbp}} := \mathcal{H}^{(0)}(\Lambda) + \varepsilon\mathcal{H}^{(1)}(\Lambda, \lambda, \eta, \xi, p, q) \qquad [27]$$

denote the Hamiltonian (eqn [8]) expressed in terms of the Poincaré symplectic variables $((\Lambda, \lambda), (\eta, \xi), (p, q))$, $\Lambda = (\Lambda_1, \ldots, \Lambda_n)$, etc.

As the number of the planets increases, the degeneracies become stronger and stronger. Furthermore, a clean reduction, such as the reduction of the nodes, is no more available if $n > 2$. To overcome these problems Herman proposed a new approach, which is described below.

Instead of Kolmogorov's nondegeneracy assumption – which says that the frequency map [13] $I \to \omega(I)$ is a local diffeomorphism – one may consider weaker nondegeneracy conditions. In particular, in Féjoz (2004), one considers nonplanar frequency maps. A smooth curve $u \in A \to \omega(u) \in \mathbb{R}^d$, where A is an open nonempty interval, is called "nonplanar" at $u_0 \in A$ if all the u-derivatives up to order $(d-1)$ at u_0, $\omega(u_0), \omega'(u_0), \ldots, \omega^{(d-1)}(u_0)$ are linearly independent in $\mathbb{R}^d$; a smooth map $u \in A \subset \mathbb{R}^p \to \omega(u) \in \mathbb{R}^d, p \le d$, is called nonplanar at $u_0 \in A$ if there exists a smooth curve $\varphi : \hat{A} \to A$ such that $\omega \circ \varphi$ is nonplanar at $t_0 \in \hat{A}$ with $\varphi(t_0) = u_0$. A S Pyartli has proved (see, e.g., Féjoz (2004)) that if the map $u \in A \subset \mathbb{R}^p \to \omega(u) \in \mathbb{R}^d$ is nonplanar at u_0, then there exists a neighborhood $B \subset A$ of u_0 and a subset $C \subset B$ of full Lebesgue measure (i.e., $\mathrm{meas}(C) = \mathrm{meas}(B)$) such that $\omega(u)$ is Diophantine for any $u \in C$. The nonplanarity condition is weaker than Kolmogorov's nondegeneracy conditions; for example, the map

$$\begin{aligned} \omega(I) &:= \partial_I\left(\frac{I_1^4}{4} + I_1^2 I_2 + I_1 I_3 + I_4\right) \\ &= \left(I_1^3 + 2I_1 I_2 + I_3, I_1^2, I_1, 1\right) \end{aligned}$$

violates both Kolmogorov's nondegeneracy and the isoenergetic nondegeneracy conditions but is nonplanar at any point of the form $(I_1, 0, 0, 0)$, since $\omega(I_1, 0, 0, 0) = (I_1^3, I_1^2, I_1, 1)$ is a nonplanar curve (at any point).

As in the three-body case, the frequency map is that associated with the averaged secular Hamiltonian

$$\begin{aligned} \mathcal{H}_{\mathrm{sec}} &:= \mathcal{H}^{(0)}(\Lambda) + \varepsilon\bar{\mathcal{H}}^{(1)} \\ \bar{\mathcal{H}}^{(1)}(\Lambda, \eta, \xi, p, q) &:= \int \mathcal{H}^{(1)} \frac{\mathrm{d}\lambda}{(2\pi)^n} \end{aligned} \qquad [28]$$

which has an elliptic equilibrium at $\eta = \xi = p = q = 0$ (as above, Λ is regarded as a parameter). It is a remarkably well-known fact that the quadratic part of $\bar{\mathcal{H}}^{(1)}$ does not contain "mixed terms," namely,

$$\begin{aligned} \bar{\mathcal{H}}^{(1)} = \bar{\mathcal{H}}_0^{(1)} &+ \varepsilon\big(\mathcal{Q}_{\mathrm{pln}}\,\eta\cdot\eta + \mathcal{Q}_{\mathrm{pln}}\,\xi\cdot\xi + \mathcal{Q}_{\mathrm{spt}}\,p\cdot p \\ &+ \mathcal{Q}_{\mathrm{spt}}\,q\cdot q + O_4\big) \end{aligned} \qquad [29]$$

where the function $\bar{\mathcal{H}}_0^{(1)}$ and the symmetric matrices $\mathcal{Q}_{\mathrm{pln}}$ and $\mathcal{Q}_{\mathrm{spt}}$ depend upon Λ while O_4 denotes terms of order 4 in (η, ξ, p, q). The eigenvalues of the matrices $\mathcal{Q}_{\mathrm{pln}}$ and $\mathcal{Q}_{\mathrm{spt}}$ are the first Birkhoff invariants of $\bar{\mathcal{H}}^{(1)}$ (with respect to the symplectic variables (η, ξ, p, q)). Let $\sigma_1, \ldots, \sigma_n$ and $\varsigma_1, \ldots, \varsigma_n$ denote, respectively, the eigenvalues of $\mathcal{Q}_{\mathrm{pln}}$ and $\mathcal{Q}_{\mathrm{spt}}$; then the frequency map for the $(1+n)$-body problem will be defined as (recall eqn [18])

$$\Lambda \to (\hat{\omega}, \varepsilon\Omega) \qquad [30]$$

with

$$\begin{aligned} \hat{\omega} &:= \left(\frac{\kappa_1}{\Lambda_1^3}, \ldots, \frac{\kappa_n}{\Lambda_n^3}\right) \\ \Omega &:= (\sigma, \varsigma) := ((\sigma_1, \ldots, \sigma_n), (\varsigma_1, \ldots, \varsigma_n)) \end{aligned} \qquad [31]$$

Herman pointed out, however, that the frequencies σ and ς satisfy two independent linear relations, namely (up to renumbering the indices),

$$\varsigma_n = 0, \qquad \sum_{i=1}^{n}(\sigma_i + \varsigma_i) = 0 \qquad [32]$$

which clearly prevents the frequency map to be nonplanar; the second relation in eqn [32] is usually

called "Herman resonance" (while the first relation is a well-known consequence of rotation invariance).

The degeneracy due to rotation invariance may be easily taken care of by considering (as in the three-body case) the $(6n-2)$-dimensional invariant symplectic manifold $\mathcal{M}_{\mathrm{ver}}$, defined by taking the total angular momentum C to be vertical, that is, $C \cdot k_1 = 0 = C \cdot k_2$. But, when $n > 2$, Jacobi's reduction of the nodes is no more available and to get rid of the second degeneracy (Herman's resonance), the authors bring in a nice trick, originally due – once more! – to Poincaré. In place of considering $\mathcal{H}_{\mathrm{nbp}}$ restricted on $\mathcal{M}_{\mathrm{ver}}$, Féjoz considers the modified Hamiltonian

$$\mathcal{H}^{\delta}_{\mathrm{nbp}} := \mathcal{H}_{\mathrm{nbp}} + \delta C_3^2, \quad C_3 := C \cdot k_3 = |C| \qquad [33]$$

where $\delta \in \mathbb{R}$ is an extra artificial parameter. By an analyticity argument, it is then possible to prove that the (rescaled) frequency map

$$(\Lambda, \delta) \to (\hat{\omega}, \sigma_1, \ldots, \sigma_n, \varsigma_1, \ldots, \varsigma_{n-1}) \in \mathbb{R}^{3n-1}$$

is nonplanar on an open dense set of full measure and this is enough to find a positive measure set of Lagrangian maximal $(3n-1)$-dimensional invariant tori for $\mathcal{H}^{\delta}_{\mathrm{nbp}}$; but, since $\mathcal{H}^{\delta}_{\mathrm{nbp}}$ and $\mathcal{H}_{\mathrm{nbp}}$ commute, a classical Lagrangian intersection argument allows one to conclude that such tori are invariant also for $\mathcal{H}_{\mathrm{nbp}}$ yielding the complete proof of Arnol'd's theorem in the general case. Notice that this argument yields $(3n-1)$-dimensional tori, which in the three-body case means five dimensional. Instead, the tori found in the section "The spatial three-body problem" are four dimensional. The point is that in the reduced phase space, the motion of the nodeline – denoted as $\psi_2(t)$ in eqn [25] – does not appear.

We conclude this discussion by mentioning that the KAM theory used in Féjoz (2004) is a modern and elegant function-theoretic reformulation of the classical theory and is based on a C^∞ local inversion theorem (F Sergeraert and R Hamilton) on "tame" Frechet spaces (which, in turn, is related to the Nash–Moser implicit function theorem; see Bost (1984–85)).

Lower Dimensional Tori

The maximal tori for the many-body problems described above are found near the elliptic equilibria given by the decoupled Keplerian motions. It is natural to ask what happens of such elliptic equilibria when the interaction among planets is taken into account. Even though no complete answer has yet been given to such a question, it appears that, in general, the Keplerian elliptic equilibria "bifurcate" into elliptic n-dimensional tori. This section presents a short and nontechnical account of the existing results on the matter (the general theory of lower-dimensional tori is, mainly, due to J K Moser and S M Graff for the hyperbolic case and V K Melnikov, H Eliasson, and S B Kuksin for the technically more difficult elliptic case; for references, see, e.g., Chierchia *et al.* (2004)).

The normal form of a Hamiltonian admitting an n-dimensional elliptic invariant torus $\mathcal{T}$ of energy E, proper frequencies $\hat{\omega} \in \mathbb{R}^n$, and "normal frequencies" $\Omega \in \mathbb{R}^p$ in a $2d$-dimensional phase space with $d = n + p$ is given by

$$N := E + \hat{\omega}_{\mathrm{r}} \cdot y + \sum_{j=1}^{p} \Omega_j \frac{\eta_j^2 + \xi_j^2}{2} \qquad [34]$$

Here the symplectic form is given by $dy \wedge dx + d\eta \wedge d\xi, y \in \mathbb{R}^n, x \in \mathbb{T}^n, (\eta, \xi) \in \mathbb{R}^{2p}; \mathcal{T}$ is then given by $\mathcal{T} := \{y = 0\} \times \{\eta = \xi = 0\}$. Under suitable assumptions, a set of such tori persists under the effect of a small enough perturbation $P(y, x, \eta, \xi)$. Clearly, the union of the persistent tori (if $n < d$) forms a set of zero measure in phase space; however, in general, n-parameter families persist.

In the many-body case considered in this article, the proper frequencies are the Keplerian frequencies given by the map $\Lambda \to \hat{\omega}(\Lambda)$ (eqn [31]), which is a local diffeomorphism of $\mathbb{R}^n$. The normal frequencies Ω, instead, are proportional to ε and are the first Birkhoff invariants around the elliptic equilibria as discussed above. Under these circumstances, the main nondegeneracy hypothesis needed to establish the persistence of the Keplerian n-dimensional elliptic tori boils down to the so-called Melnilkov condition:

$$\Omega_j \neq 0 \neq \Omega_i - \Omega_j, \quad \forall j \neq i \qquad [35]$$

Such condition has been checked for the planar three-body case in Féjoz (2002), for the spatial three-body case in Biasco *et al.* (2003) and for the planar n-body case in Biasco *et al.* (2004). The general spatial case is still open: in fact, while it is possible to establish lower-dimensional elliptic tori for the modified Hamiltonian $\mathcal{H}^{\delta}_{\mathrm{nbp}}$ in [33], it is not clear how to conclude the existence of elliptic tori for the actual Hamiltonian $\mathcal{H}_{\mathrm{nbp}}$ since the argument used above works only for Lagrangian (maximal) tori; on the other hand, the direct asymptotics techniques used in Biasco *et al.* (2003) do not extend easily to the general spatial case.

Clearly, the lower-dimensional tori described in this section are not the only ones that arise in n-body dynamics. For more lower-dimensional tori in the planar three-body case, see Féjoz (2002).

Physical Applications

The above results show that, in principle, there may exist "stable planetary systems" exhibiting quasiperiodic motions around coplanar, circular Keplerian trajectories – in the Newtonian many-body approximation – provided the masses of the planets are much smaller than the mass of the central star.

A quite different question is: in the Newtonian many-body approximation, is the solar system or, more in generally, a solar subsystem stable?

Clearly, even a precise mathematical reformulation of such a question might be difficult. However, it might be desirable to develop a mathematical theory for important physical models, taking into account observed parameter values.

As a very preliminary step in this direction, consider one of the results of Celletti and Chierchia (see Celletti and Chierchia (2003), and references therein).

In Celletti and Chierchia (2003), the (isolated) subsystem formed by the Sun, Jupiter, and asteroid Victoria (one of the main objects in the Asteroidal belt) is considered. Such a system is modeled by an order-10 Fourier truncation of the RPC3BP, whose Hamiltonian has been described in the section "Kolmogorov's theorem and the RPC3BP (1954)." The Sun–Jupiter motion is therefore approximated by a circular one, the asteroid Victoria is considered massless, and the motions of the three bodies are assumed to be coplanar; the remaining orbital parameters (Jupiter/Sun mass ratio, which is approximately 1/1000; eccentricity and semimajor axis of the osculating Sun–Victoria ellipse; and "energy" of the system) are taken to be the actually observed values. For such a system, it is proved that there exists an invariant region, on the observed fixed energy level, bounded by two maximal two-dimensional Kolmogorov tori, trapping the observed orbital parameters of the osculating Sun–Victoria ellipse.

As mentioned above, the proof of this result is computer assisted: a long series of algebraic computations and estimates is performed on computers, keeping a rigorous track of the numerical errors introduced by the machines.

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See also: Averaging Methods; Diagrammatic Techniques in Perturbation Theory; Gravitational *N*-Body Problem (Classical); Hamiltonian Systems: Stability and Instability Theory; Hamilton–Jacobi Equations and Dynamical Systems: Variational Aspects; Korteweg–de Vries Equation and Other Modulation Equations; Stability Problems in Celestial Mechanics; Stability Theory and KAM.

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Kinetic Equations

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Introduction

In most physical cases, the evolution of a system of N indistinguishable interacting particles $X_N = (x_1, x_2, \ldots, x_N)$ with velocities $V_N = (v_1, v_2, \ldots, v_N)$ is described by a Hamiltonian system

$$\frac{\mathrm{d}X_N}{\mathrm{d}t} = \frac{\partial H(X_N, V_N)}{\partial V_N}$$
$$\frac{\mathrm{d}V_N}{\mathrm{d}t} = -\frac{\partial H(X_N, V_N)}{\partial X_N} \qquad [1]$$

in the phase space $\boldsymbol{R}_X^{dN} \times \boldsymbol{R}_V^{dN}$. When N becomes large, it is natural to consider replacing the above discrete phase space by a continuous phase space of dimension $1 \le d \le 3$, $\boldsymbol{R}_x^d \times \boldsymbol{R}_v^d$ and to introduce a measure $f(x, v, t)$ that describes the density of particles which, at the point $x \in \boldsymbol{R}^d$ and at time t, have velocity v. This measure may also be interpreted as a generalization of the empirical measure

$$\mu_N(t) = \frac{1}{N} \sum_{1 \le i \le N} \delta_{x_i(t), v_i(t)}$$

defined in the phase space $\boldsymbol{R}_x^d \times \boldsymbol{R}_v^d$ by the above system of N particles. In this way, one constructs a link between the microscopic and the macroscopic descriptions. The macroscopic physical quantities are, for instance, the first moments of this density:

$$\rho(x,t) = \int_{\boldsymbol{R}_v^d} f(x, v, t)\mathrm{d}v \text{ (density)}$$
$$\rho(x,t)u(x,t) = \int_{\boldsymbol{R}_v^d} v f(x, v, t)\mathrm{d}v \text{ (momentum)}$$
$$\rho(x,t)E(x,t) = \int_{\boldsymbol{R}_v^d} \frac{|v|^2}{2} f(x, v, t)\mathrm{d}v \text{ (energy)}$$

Kinetic theory studies the intermediate stage shown in **Figure 1**.

Its first successes were related to classical thermodynamics and in particular to the molecular hypothesis. The contributions of Maxwell (1860, 1872) and of Boltzmann (1867) led to the "Boltzmann" equation, described in the companion article of Mario Pulvirenti (*see* Boltzmann Equation (Classical and Quantum)). In 1905, Lorentz used the same point of view to describe the motion of electrons in a metal. However, the different physical context leads to some basic differences between the Boltzmann equation and the Lorentz equation. The Boltzmann equation is derived under the assumption that the driving forces result from collisions between pairs of molecules. Therefore, the problem is nonlinear with a quadratic nonlinearity. In the Lorentz model the driving force is the interaction of the electrons with the atoms of the metal, which remain fixed. Collisions between electrons are ignored, so that the Lorentz equation is linear.

Hamiltonian Systems $\xrightarrow{1}$ Kinetic equations $\xrightarrow{2}$ Macroscopic equations

Figure 1 Illustration of the role of kinetic equations in linking microscopic and macroscopic properties.

The most general form of a kinetic equation is as follows:

$$\partial_t f(x, v, t) + \nabla_v H_f \cdot \nabla_x f(x, v, t)$$
$$- \nabla_x H_f \cdot \nabla_v f(x, v, t) = C(f) \qquad [2]$$

The term $C(f)$ represents the effect of interactions either between particles or with the background. Without this term, the eqn [2] is reduced to the classical Liouville equation

$$\partial_t f(x, v, t) + \nabla_v H_f \cdot \nabla_x f(x, v, t)$$
$$- \nabla_x H_f \cdot \nabla_v f(x, v, t) = 0 \qquad [3]$$

which says that the function f is transported by the flow of the Hamiltonian $H_f(x, v)$. This Hamiltonian depends on the model and may involve the unknown function f itself. In the simplest case $H(x, v) = |v|^2/2$, eqn [3] and its solutions are given by

$$\partial_t f(x, v, t) + v \cdot \nabla_v f(x, v, t) = 0$$
$$f(x, v, t) = f(x - vt, v, 0) \qquad [4]$$

Nowadays kinetic equations appear in a variety of sciences and applications, such as astrophysics, aerospace engineering, nuclear engineering, particle–fluid interactions, semiconductor technology, social sciences, and biology, for example in chemotaxis and immunology.

They are used first to model phenomena and then to obtain a qualitative and quantitative description of situations involving sufficiently many particles so as to prohibit any computation at the level of particles, and yet the medium is still too rarefied to allow the use of macroscopic equations. As detailed in the next section, a macroscopic description requires that the function $f(x, v, t)$ be close to local thermodynamical equilibrium. For classical and quantum Boltzmann equations (*see* Boltzmann

Equation (Classical and Quantum)) these equilibria are either Maxwellian, Bose–Einstein, or Fermi–Dirac distributions.

Several effects, especially the influence of the boundary, may prevent the system from reaching local thermodynamical equilibrium and, therefore, even in macroscopic descriptions, kinetic equations may still be used to take into account the effect of the boundary. In this case, the term "Knudsen boundary layer" is currently used.

Finally, one should keep in mind that there exist some macroscopic phenomena which cannot be deduced from the corresponding microscopic physics by the mediation of a kinetic equation. Once again, returning to the companion article (*see* Boltzmann Equation (Classical and Quantum)) one observes that, since the only equilibria are Maxwellian, the macroscopic equations are those describing perfect gases. A real gas with a nontrivial van der Waals law is "too dense" to be explained by this theory. The alternative seems to go directly from the microscopic direction to the macroscopic description. This is a subject which is still under investigation and for which the reader may consult Olla *et al.* (1993).

Kinetic Equations Entropy and Irreversibility

At the level of particles, the basic laws of physics are reversible. Yet these same laws are not reversible when seen at the level of a macroscopic description. This lack of reversibility is measured by the decay of entropy (mathematicians prefer convex functions; therefore, the mathematical entropy considered in this contribution is the negative of the physical entropy, and with irreversibility it decays). The kinetic equations lie in between, as shown in **Figure 1**; the decay of entropy should appear along one of the two arrows of this diagram.

Since the appearance of irreversibility is related to loss of information and averaging, it should be driven by a "mixing" process.

In general two mechanisms are responsible for such effects:

1. an ergodic or a relaxation mechanism by which a process averages itself; and
2. the introduction of some external random parameter. Observable quantities are then defined as averages over that parameter.

It seems important to compare these two "processes." This will be illustrated below with the most classical examples of the theory.

The Diffusion Limit for the Neutron Transport Equation

Equations very similar to the one introduced by Lorentz are used to describe the interaction of neutrons with atoms in a nuclear reactor: this is the reason why these types of equations are often called neutron transport equations. An important issue is the derivation of a macroscopic diffusion equation. Assuming that neutrons are not subject to acceleration effects, considering the problem with constant modulus of velocity ($|v| = 1$), introducing a "small" parameter ϵ which here corresponds to the absorption of the medium, one can study the following simplified model:

$$\epsilon\partial_t f_\epsilon + v\cdot\nabla_x f_\epsilon + \frac{\sigma(x)}{\epsilon}\left(f_\epsilon - \int_{|v'|=1} k(v,v')f_\epsilon(v')\mathrm{d}v'\right) = 0 \qquad [5]$$

In [5] one assumes, for the kernel $k(v,v')$, the following properties:

$$\forall v,\ v',\quad k(v,v') = k(v',v),\ \ 0 < k(v,v')$$
$$\int_{|v'|=1} k(v,v')\mathrm{d}v = 1 \qquad [6]$$

and denotes by K the operator

$$f \mapsto Kf = \int_{|v'|=1} k(v,v')f(v')\mathrm{d}v'$$

In the simplest case (say without boundary) eqn [5] is well-posed both for positive and negative time but hypothesis [6] has the following important consequences:

1. For positive time, it defines, for each $\epsilon > 0$, a contraction semigroup in any L^p space and, therefore, the sequence of solutions or a subsequence thereof converges, say weakly, to a limit $f(x, v, t)$.
2. One also observes that $v \mapsto 1$ is (up to a multiplicative constant) the only solution of the equation

$$f - Kf = f(v) - \int_{|v'|=1} k(v,v')f(v')\mathrm{d}v = 0 \qquad [7]$$

Therefore, the ϵ^{-1} in front of the collision term forces the limit $f(x, v, t)$ to be independent of v. In this simple problem, this is the thermodynamical equilibrium.

Dividing by ϵ and integrating over $|v| = 1$ gives the relation

$$\partial_t \int_{|v|=1} f_\epsilon(x,v,t)\mathrm{d}v + \nabla_x \frac{1}{\epsilon}\int_{|v|=1} v f_\epsilon(x,v,t)\mathrm{d}v = 0 \qquad [8]$$

Now using the Fredholm alternative implies the existence and uniqueness of a function $v \mapsto \beta(v)$ such that

$$\beta(v) - \int_{|v'|=1} k(v,v')\beta(v')\mathrm{d}v' = v, \int_{|v'|=1} \beta(v')\mathrm{d}v' = 0 \qquad [9]$$

Multiply eqn [5] by $\beta(v)$ and integrate over $|v| = 1$ to obtain

$$\begin{aligned}\lim_{\epsilon\to 0}\frac{\sigma(x)}{\epsilon}\int_{|v|=1}((I-K)\beta)(v)f_\epsilon(x,v,t)\mathrm{d}v &= \lim_{\epsilon\to 0}\frac{\sigma(x)}{\epsilon}\int_{|v|=1}\beta(v)(I-K)f_\epsilon(x,v,t)\mathrm{d}v \\ &= -\lim_{\epsilon\to 0}\nabla_x\int_{|v|=1}\beta(v)\otimes v f_\epsilon(x,v,t)\mathrm{d}v \qquad [10]\end{aligned}$$

Since the operator $(I - K)$ is self-adjoint non-negative, with 0 as the leading eigenvalue, the matrix

$$D = \int_{|v|=1}\beta(v)\otimes v\mathrm{d}v = \int_{|v|=1}\beta(v)\otimes(I-K)\beta(v)\mathrm{d}v$$

is positive definite, and one finally obtains the diffusion equation

$$\partial_t f - \nabla_x\left(\frac{D}{\sigma(x)}\nabla_x f\right) = 0 \qquad [11]$$

The above derivation is an example of what is called the "moments method." It is implicit even in the papers of Maxwell. It has been systematically used in several domains:

- To understand the relation between the Boltzmann equation and the Euler and Navier–Stokes equations (Golse 2005);
- To compute the critical size of a nuclear assembly. One shows that this size is well approximated by the size of the domain for which the Laplacian, with appropriate boundary conditions, has leading eigenvalue 0. It is for the spectral analysis of this problem that the averaging lemma (see the section "Some specific mathematical tools") was derived.
- To analyze the macroscopic limit for the solution of the radiative transfer equations, which describe the propagation of the intensity of photons in a large class of phenomena ranging from stellar atmospheres to the cooling of glass, including optical tomography in biomedical imaging. In a simplified form, the so-called "grey model," these equations can be reduced to

$$\begin{aligned}&\epsilon\partial_t I_\epsilon(x,v,t) + v\cdot\nabla_x I_\epsilon(x,v,t) \\ &+\frac{1}{\epsilon}\sigma\Big(\frac{1}{4\pi}\int_{|v'|=1} I_\epsilon(x,v',t))\mathrm{d}v'\Big)\Big(I_\epsilon(x,v,t) \\ &-\frac{1}{4\pi}\int_{|v'|=1} I_\epsilon(x,v',t))\,\mathrm{d}v'\Big) = 0 \qquad [12]\end{aligned}$$

In contrast to the previous example, the problem is, in many cases, nonlinear. The opacity σ is a positive function that depends on the intensity I_ϵ through

$$\tilde{I}(x,t) = \frac{1}{4\pi}\int_{|v'|=1} I_\epsilon(x,v',t)\,\mathrm{d}v'$$

and which goes to ∞ with $\tilde{I}_\epsilon$ going to zero. The moments method can be applied with the averaging lemma, and one shows that the limit of I_ϵ is a function that is independent of v and satisfies the following degenerate parabolic equation:

$$\partial_t I - \nabla_x\left(\frac{1}{3\sigma(I)}\nabla_x I\right) = 0 \qquad [13]$$

This equation is similar to the one obtained in the description of porous media and contains the following information: for initial data $I(x,0)$ with compact support, in contrast to the behavior of solutions of the standard diffusion equation, the solution $I(x,t)$ remains compactly supported in x. The boundary of this support is the thermal front and for a finite time, up to saturation (by water in porous media, by reacted deuterium in laser-confined fusion), this front remains fixed.

What made the analysis of the above macroscopic limit simple was the existence of an $\epsilon > 0$ dependent process which, for vanishing ϵ, forces the solution to converge to a "thermodynamical" equilibrium. The irreversibility was already present in the first arrow of **Figure 1**. This is what made the analysis of the second arrow simple. The subtleties of the appearance of the irreversibility in the first arrow may be well explained by the next examples.

The Linear Billiard Model

In the absence of an external electric field, the model proposed by Lorentz could be viewed as a limit of a system of particles evolving freely between spherical obstacles and reflecting on these obstacles according to the law of geometric optics. Along these lines, two types of results have been proved in two space variables.

In 1973, Gallavotti considered the case where the obstacles are randomly spaced under a Poisson configuration and proved the following theorem:

Theorem 1 *Consider obstacles(balls) of radius ϵ and center c_i. Assume that the probability of finding exactly N such obstacles in a bounded measurable set $\Lambda \subset \mathbf{R}^2$ is given by the "Poisson law"*

$$P(\mathrm{d}\mathbf{c}_N) = \mathrm{e}^{-\mu_\epsilon|\Lambda|}\frac{\mu_\epsilon^N}{N!}\,\mathrm{d}c_1\,\mathrm{d}c_2\cdots\mathrm{d}c_N \qquad [14]$$

with

$$\mathbf{c}_N = c_1, c_2, \ldots, c_N \quad \text{and} \quad \mu_\epsilon = \frac{\mu}{\epsilon} \qquad [15]$$

Denote by $\mathbf{E}^\epsilon$ the expectation with respect to the above Poisson distribution. For given ϵ and $\mathbf{c}_N$ introduce

$$\mathrm{O}_{\mathbf{c}_N,\epsilon} = \mathbf{R}^2 \backslash \cup_{1\le i\le N}\{|x-c_i|\le\epsilon\} \qquad [16]$$

and $f_{\mathbf{c}_N,\epsilon}$, the solution of the problem

$$\partial_t f_{\mathbf{c}_N,\epsilon}(x,v,t) + v\cdot\nabla_x f_{\mathbf{c}_N,\epsilon}(x,v,t) = 0 \quad \text{in } \mathrm{O}_{\mathbf{c}_N,\epsilon}\times S^1 \qquad [17]$$

with specular reflection on the boundary and v-independent initial data:

$$f_{\mathbf{c}_N,\epsilon}(x,v,0) = \phi(x) \quad \text{in } \mathrm{O}_{\mathbf{c}_N,\epsilon}\times S^1 \qquad [18]$$

Then

$$h_\epsilon(x,t,\Omega) = \mathbf{E}^\epsilon[f_{\mathbf{c}_N,\epsilon}] \qquad [19]$$

converges weakly for $t\ge 0$ to the solution of the transport equation

$$\partial_t f(x,v,t) + v\cdot\nabla f(x,v,t) + \mu\left[2f(x,v) - \frac{1}{4}\int_S f(x,v')|v-v'|\mathrm{d}v'\right] = 0 \qquad [20]$$

$$f(x,v,0) = \phi(x) \quad \text{in } \mathbf{R}^2\times S^1 \qquad [21]$$

The situation is completely different when the obstacles are periodically spaced, a situation which seems closer to Lorentz's original idea. Golse (2003) (and previous contributions quoted in this article) obtained the following result:

Theorem 2 *Assume that the obstacles are periodically spaced and conveniently scaled, defining the domain*

$$\mathrm{O}_\epsilon = \mathbf{R}^2 \backslash \bigcup_{j\in\mathbf{Z}^2}\{x, |x-\epsilon j|\le\epsilon^2\} \qquad [22]$$

Then there exists a family of continuous uniformly bounded initial data such that no subsequence extracted from the family of solutions of

$$\partial_t f_\epsilon + v\cdot\nabla_x f_\epsilon = 0 \quad \text{in } \mathrm{O}_\epsilon\times S^1 \qquad [23]$$

with specular reflections on the boundary, converges to solutions of equations of the type [20].

This pathology is related to the existence of particles that can travel freely for a very long time before meeting the obstacles, and the proof with some arithmetic (Diophantine approximations and continued fractions) relies on the analysis of such trajectories.

A comparison between the Theorems 1 and 2 shows that the ergodic property of the free flow on the periodic lattice is not strong enough to lead to a collisional kinetic equation unless some complementary randomness is introduced.

The examples of this section should be compared with the rigorous derivation of the Boltzmann equation by Lanford (*see* Boltzmann Equation (Classical and Quantum)). The reader should observe that this derivation corresponds to the same type of scaling (finite mean free path). However, no extra randomness is needed in this case. The proof uses the fact that configurations leading only to a finite number of binary collisions are of full measure. This corresponds to an ergodicity property which is enforced by the fact that the problem is genuinely nonlinear.

Mean-Field Scaling and Vlasov Equations

The neutron transport equation is devoted to the interaction with obstacles and the Boltzmann equation to binary collisions. A simpler situation from the mathematical point of view corresponds to the case where each particle is under the action of the average of all other particles. Then the name "mean field limit" is used. The simplest example is the derivation of a Vlasov-type equation from a system of N classical particles interacting with a C^2 potential $V(|x|)$. The following Hamiltonian is used:

$$H(x_1,\ldots,x_N,v_1,\ldots,v_N) = \sum_{1\le k\le N}\frac{|v_k|^2}{2} + \frac{1}{2N}\sum_{1\le l\ne k\le N} V(|x_k-x_l|) \qquad [24]$$

and the name mean-field scaling is related to the factor N^{-1} before the potential. Assuming that the particles are undistinguishable, one introduces the joint probability density $F_N \equiv F_N(x_1,\ldots,x_N,$

$v_1, \ldots, v_N)$ in the N-particle phase space, which satisfies the Liouville equation

$$\partial_t F_N + \{H_N, F_N\} := \partial_t F_N + \sum_{1\le k\le N} \Big(v_k \nabla_{x_k} F_N - \frac{1}{2N} \sum_{1\le l\ne k\le N} \nabla_{x_k}(V(|x_k - x_l|)) \times \nabla_{v_k} F_N \Big) = 0 \qquad [25]$$

From [25], with the notations

$$X_n = (x_1, \ldots, x_n), \quad V_n = (v_1, \ldots, v_n)$$
$$X_N^n = (x_{n+1}, \ldots, x_N), \quad V_N^n = (x_{n+1}, \ldots, x_N)$$

one deduces an infinite hierarchy of equations for the marginals

$$F_N^n(X_n, V_n, t) = \int f_N(X_N, V_N, t)\mathrm{d}X_N^n\, \mathrm{d}V_N^n$$
$$\text{for } 1 \le n \le N, \ F_N^n \equiv 0 \text{ for } N < n:$$

$$\partial_t F^n(X_n, V_n, t) + \sum_{1\le i\le n} v_n \nabla_{x_i} F_N^n(X_n, V_n, t) - \frac{1}{N} \sum_{1\le i<j\le n} \nabla_{v_i}(\nabla_{x_i} V(|x_i - x_j|) F_N^n(X_n, V_n, t)) - \frac{N-n}{N}\Big(\sum_{1\le i\le n} \nabla_{v_i} \iint \nabla_{x_i} V(|x_i - x^*|) \times F_N^{n+1}(X_n, V_n, x^*, v^*, t)\mathrm{d}x^* \mathrm{d}v^* \Big) = 0 \qquad [26]$$

Letting N go to infinity, one obtains "formally," for the distribution functions,

$$F^n = \lim_{N\to\infty} F_N^n$$

the Vlasov hierarchy:

$$\partial_t F^n(X_n, V_n, t) + V_n \cdot \nabla_{X_n} F^n(X_n, V_n, t) - \sum_{1\le i\le n} \nabla_{v_i} \Big(\iint \nabla_{x_i} V(|x_i - x^*|) \times F_N^{n+1}(X_n, V_n, x^*, v^*, t)\mathrm{d}x^* \mathrm{d}v^* \Big) = 0 \qquad [27]$$

Observe that for any density $F(x, v, t)$ that satisfies

$$\iint F(x, v, t)\mathrm{d}x\, \mathrm{d}v = 1, \quad F(x, v, t) \ge 0 \qquad [28]$$

and is a solution of the V potential Vlasov equation:

$$\partial_t F(x, v, t) + v \cdot \nabla_x F(x, v, t) - \Big(\iint \nabla_x V(|x - x^*|) F(x^*, v^*)\mathrm{d}x^* \mathrm{d}v^* \Big) \times \nabla_v F(x, v, t) = 0 \qquad [29]$$

the factorization formula

$$F^n(X_n, V_n, t) = \prod_{1\le i\le n} F(x_i, v_i, t) \qquad [30]$$

defines a solution of the above Vlasov hierarchy.

A uniqueness argument implies that any solution of the Vlasov hierarchy which is factorized at time zero will remain factorized at any subsequent time. Such a property, also observed for the hierarchy leading to the Boltzmann equation, is called the propagation of chaos. To make the proof rigorous, one has to analyze the limiting process in the hierarchy and prove the uniqueness of the solution of the infinite hierarchy. For a smooth potential, this has been done by Braun and Hepp in 1977 and by Spohn in 1981. An interesting approach consists, following Dobrushin, in introducing the Wasserstein distance; see Golse (2003) for a detailed exposition.

In the case of the Vlasov–Poisson equation [29] with $V(|x|) = 1/4\pi|x|$ the potential turns out to be too singular for the above derivation. In particular, the corresponding solution of the N-particle problem is not uniformly defined. However, for the corresponding equation (and for variants thereof, including the effect of the magnetic field, the Vlasov–Maxwell system) a series of mathematical results concerning existence and stability of solutions have been obtained. An excellent recent exposition of these results can be found in the book of Glassey (1996).

Equation [29] as well as the original system turns out to be fully reversible. Neither irreversibility nor averaging has appeared in the limit process which corresponds to the first arrow of **Figure 1**; this is due to the "weak coupling." Therefore, irreversibility should now appear on the second arrow. Integrating eqn [29] with respect to v gives the relation (often called Fick's law):

$$\partial_t \rho(x, t) + \nabla_x \int v F(x, v, t)\mathrm{d}v = 0 \qquad [31]$$

But now expressing the current $j = \int vF(x, v, t)\mathrm{d}v$ in terms of macroscopic variables turns out to be a difficult issue in the absence of a "relaxation" effect. Up to now there has been no derivation of such macroscopic equations from first principles.

The same type of problems exist for the two-dimensional Euler equation, which is in some sense very similar to the Vlasov equation. It has been observed that these equations develop for "turbulent initial data" a kind of "mixing process" leading to coherent structures that would play the role of thermodynamical equilibrium (in the absence of relaxation). The Jupiter red spot is the most

well-known example of such a structure. These coherent structures are obtained by maximizing an entropy which does not come directly from the dynamics but which is inspired by similar problems in statistical mechanics. Finally, one has to take into account in this construction the existence of an infinite set of conserved quantities: for each regular function G, vanishing at infinity, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\iint G(F(x,v,t))\mathrm{d}x\,\mathrm{d}v = 0$$

This approach was already started by Onsager in 1945 and pursued by many scientists. A recent reference is the article of Chavanis and Sommeria (1998).

Derivation of Kinetic Equations from the Schrödinger Equation

Oscillatory solutions of the Schrödinger equation, with wavelength of the order of the Planck constant, tend to behave like particles. This is described in detail by different tools of high-frequency approximation. In particular, the limit of the Wigner transform of the density $\psi(x,t)\otimes\overline{\psi}(y,t)$:

$$W(x,\xi,t) = \frac{1}{(2\pi)^{3d}}\int_{R^{3d}} \mathrm{e}^{-\mathrm{i}\xi y}\psi\left(x+\frac{\hbar y}{2},t\right) \otimes\overline{\psi}\left(x-\frac{\hbar y}{2},t\right)\mathrm{d}y \quad [32]$$

is a solution of a Liouville equation. Therefore, one should expect that in the presence of "many" obstacles ("many potentials") the limit should be given by a kinetic equation. As shown by the previous section the introduction of randomness seems compulsory in reaching this goal.

Consider a big cube $\Lambda = \Lambda_L$ of size L in $\boldsymbol{R}^3$. Let $\omega = (x_\alpha), \alpha = 1,2,\ldots,N$ denote the configuration of random obstacles distributed uniformly in Λ. The density of obstacles is $\rho = N/L^3$ and the expectation with respect to this uniform measure is denoted by

$$E := \prod_{1\le\alpha\le N}\left(L^{-d}\int \mathrm{d}x_\alpha\right)$$

With $V(|x|)$ a smooth, short-range potential, the random potential created by the obstacles is

$$V_\omega(x) = \sum_{1\le\alpha\le N} V(|x-x_\alpha|)$$

then one of the typical results (low-density limit, which corresponds to the quantum version of Gallavotti classical result) obtained, reads as follows:

Theorem 3 (Erdös and Yau 1988) *Assume that the density of obstacles is $\rho = \rho_0\epsilon$ with a fixed ρ_0. Denote by $\psi^\epsilon_\omega(t)$ the solution of the Schrödinger equation*

$$\mathrm{i}\partial_t\psi^\epsilon_\omega = -\tfrac{1}{2}\Delta_x\psi^\epsilon_\omega + V_\omega\psi^\epsilon_\omega \quad [33]$$

with initial condition localized and oscillating at the scale ϵ, that is, with h and S smooth

$$\psi^\epsilon_\omega(0) = \epsilon^{3/2}h(\epsilon x)\exp\left(\mathrm{i}\frac{S(x)}{\epsilon}\right) \quad [34]$$

Consider the density matrix $\rho^\epsilon_\omega(t,x,y) = \psi^\epsilon_\omega(t,x)\otimes\overline{\psi}^\epsilon_\omega(t,y)$ and its Wigner transform

$$W^\epsilon_\omega(x,\xi,t) = \frac{1}{(2\pi)^3}\int_{R^3}\mathrm{e}^{-\mathrm{i}\xi y}\rho^\epsilon_\omega\left(t,x+\frac{\epsilon y}{2},x-\frac{\epsilon y}{2}\right)\mathrm{d}y \quad [35]$$

Then for any $t>0, EW^\epsilon_\omega(t)$ converges weakly with ϵ going to zero to a solution $F(t)$ of the kinetic equation

$$\partial_t F(t,x,\xi) + \xi\cdot\nabla_x F(t,x,\xi) = \int |T(\xi,\xi')|^2\delta(|\xi|^2-|\xi'|^2)(F(t,x,\xi') - F(t,x,\xi))\mathrm{d}\xi' \quad [36]$$

where T is the amplitude of the scattering operator associated to the Schrödinger equation with the short range potential V.

The proof uses several ingredients including scattering theory with expansion in term of Dyson series; see Erdös and Yau (1998).

Semiconductor Modeling

In modern computers, the electronic devices are so small that the electric current may have no space/time to reach a thermodynamical equilibrium. Therefore, this turns out to be a field where the kinetic equations are the most naturally used. Details of what can be deduced from a mathematical analysis can be found in Poupaud (1994). The equations involve the distribution of electrons $f_\mathrm{e}(x,k,t)$ and holes $f_\mathrm{h}(x,k,t)$ and have the following form:

$$\epsilon\partial_t f_\mathrm{e}(t,x,k) + v_\mathrm{e}(k)\nabla_x f_\mathrm{e}(t,x,k) + \frac{q}{\hbar}\nabla_x U(t,x)\cdot\nabla_k f_\mathrm{e}(t,x,k) = \frac{1}{\epsilon}(Q_\mathrm{e}(f_\mathrm{e})(t,x,k) + R_e(f_\mathrm{e},f_\mathrm{h})(t,x,k)) \quad [37]$$

$$\epsilon\partial_t f_\mathrm{h}(t,x,k) + v_\mathrm{h}(k)\nabla_x f_\mathrm{h}(t,x,k) - \frac{q}{\hbar}\nabla_x U(t,x)\cdot\nabla_k f_\mathrm{h}(t,x,k) = \frac{1}{\epsilon}Q_\mathrm{h}(f_\mathrm{h})(t,x,k) + R_\mathrm{h}(f_\mathrm{h},f_\mathrm{e})(t,x,k) \quad [38]$$

The variable k ranges over a torus B of $\boldsymbol{R}^3$ which, in physics books, carries the name of Brillouin zone. The velocities of propagation of electrons and holes are determined in terms of the energy band by the formula

$$v_{\mathrm{e,h}} = \frac{1}{\hbar}\nabla_k E_{\mathrm{e,h}}(k) \qquad [39]$$

The potential U is determined in terms of the doping profile $C(x)$, the conductivity ϵ_r, and the density of electrons and holes according to the formula

$$-\Delta_x U(t,x) = \frac{q}{\epsilon_r}\left(C(x) - \frac{1}{|B|}\int_B f_{\mathrm{e}}(t,x,k)\mathrm{d}k + \frac{1}{|B|}\int_B f_{\mathrm{h}}(t,x,k)\mathrm{d}k\right) \qquad [40]$$

Finally $Q_{\mathrm{e,h}}$ and $R_{\mathrm{e,h}}$ are binary integral operators in the variable $k \in B$ which model collisions and generation–recombination processes. Concerning the "mathematical approach" the situation is as follows.

The relations [39] can be deduced from the high-frequency analysis of the solution of the Schrödinger equation

$$\mathrm{i}\hbar\partial_t\psi = -\frac{\hbar^2}{2}\Delta\psi + V\Big(\frac{x}{\hbar}\Big)\psi \qquad [41]$$

with V a periodic potential constructed on the dual lattice of B. The method uses the Bloch decomposition of the solution and the Wigner series (Poupaud 1994). No mathematical derivation of the collisions operator is currently available. The situation should be compared to what is said in the section "Derivation of kinetic equations from the Schrödinger equation," but in a much more complicated setting.

On the other hand, the collision operators $Q_{\mathrm{e,h}}$ and $R_{\mathrm{e,h}}$, as given by phenomenological arguments, have enough good relaxation properties to allow a rigorous limit of the system [37]–[38] for ϵ going to zero (Poupaud 1994). This leads to the justification of the so-called drift–diffusion models and to the possibility of constructing correctors (with respect to ϵ) and to treating the effect of heterojunctions by boundary layer analysis.

Some Specific Mathematical Tools

Few proofs were given in the above exposition and details would not be suitable for a review article. However, the mathematical approach to kinetic equations has generated some new tools, and it may be useful to give the most prominent ones.

The Averaging Lemma

Compactness results appear in spectral theory and in the construction of solutions of nonlinear equations (whenever strong convergence is needed for the limit). Being hyperbolic, the transport operator $v \cdot \nabla_x$ propagates singularities along characteristics. Therefore, at first sight it seems hopeless that one might obtain any regularizing effect from the free streaming part of a kinetic model. The key to obtaining regularizing effects from the transport operator $v \cdot \nabla_x$ is to seek those effects not on the number density itself, but on velocity averages thereof; in other words, on the macroscopic densities.

Here is the prototype of all velocity averaging results.

Theorem 4 *Let F_ϵ be a bounded family in $L^2(\boldsymbol{R}^d \times \boldsymbol{R}^d)$. Assume that the family $v \cdot \nabla_x F_\epsilon$ is also bounded in $L^2(\boldsymbol{R}^d \times \boldsymbol{R}^d)$. Then, for each $\phi \in L^2(\boldsymbol{R}^d)$, the family of moments $\rho_\epsilon(x)$ defined by*

$$\rho_\epsilon(x) = \int_{\boldsymbol{R}^d} F_\epsilon(x,v)\phi(v)\mathrm{d}v$$

is relatively compact in $L^2(\boldsymbol{R}^d)$.

For the proof one starts with the expression $G_\epsilon = F_\epsilon + v \cdot \nabla_x F_\epsilon$ takes the Fourier transform with respect to x of this relation and writes for $\hat{\rho}_\epsilon(\xi)$ the expression

$$\hat{\rho}_\epsilon = \int_{\boldsymbol{R}^d} \frac{\hat{G}_\epsilon(\xi,v)\phi(v)\mathrm{d}v}{1 + \mathrm{i}v.\xi} \qquad [42]$$

Then use the Cauchy–Schwarz inequality to obtain

$$|\hat{\rho}_\epsilon|^2 \le \left(\int_{\boldsymbol{R}^d} \frac{|\phi(v)|^2\mathrm{d}v}{1 + |v \cdot \xi|^2}\right)\int_{\boldsymbol{R}^d}|G_\epsilon(\xi,v)|^2\mathrm{d}v \qquad [43]$$

and complete the proof by standard arguments.

The averaging lemma was first observed by Agoshkov (1984) for abstract results concerning the regularity of solutions of kinetic equations in domains with boundary. Independently, it was rediscovered in the improved form given above by Golse, Perthame, and Sentis (1985) and used for the spectral theory in the diffusion approximation. The extension to $L^p, p > 1$, spaces and to L^1 (with use of entropy estimate) were instrumental in proving the validity of the Rosseland approximation for the radiative transfer equations and for the proof of existence by Lions and Di Perna of renormalized solutions of the Boltzmann equation. A more refined result needs to be used to establish the incompressible limit of the solutions of the Boltzmann equations; see Golse (2005) for details and a complete list of references.

The Dispersive Property

Consider for the solutions in $\mathbf{R}_x^d \times \mathbf{R}_v^d$ of the elementary kinetic equations

$$\partial_t f + v \cdot \nabla_x f = 0, \quad f(x, v, 0) = f^0(x, v) \qquad [44]$$

the local density

$$\rho(x, t) = \int_{\mathbf{R}_v^d} f(x, v, t) \mathrm{d}v \qquad [45]$$

From the relation

$$\begin{aligned} |\rho(x,t)| &= \int_{\mathbf{R}_v^d} f(x,v,t)\mathrm{d}v \\ &= \int_{\mathbf{R}_v} f^0(x - vt, v, t)\mathrm{d}v \\ &\leq \int_{\mathbf{R}^d} \sup_{w \in \mathbf{R}^d} |f^0(x - vt, w)|\mathrm{d}v \end{aligned} \qquad [46]$$

deduce with an elementary change of variable the following estimate, which carries the name of dispersion lemma,

$$|\rho(x,t)| \leq \frac{1}{|t|^d} \|f^0\|_{L^1(\mathbf{R}_x^d; L^\infty(\mathbf{R}_v^d))} \qquad [47]$$

From interpolation and duality arguments follows:

Proposition 1 *The macroscopic density ρ defined by* [45] *satisfies the inequality*

$$\|\rho\|_{L^q(\mathbf{R}_t; L^p(\mathbf{R}_x^d))} \leq C(d) \|f^0\|_{L^a(\mathbf{R}^{2d})} \qquad [48]$$

for any choice of real numbers a, p, and q such that

$$\begin{aligned} &1 \leq p < \frac{d}{d-1}, \quad \frac{2}{q} = \frac{d}{1 - \frac{1}{p}} \\ &1 \leq a = \frac{2p}{p+1} < \frac{2d}{2d-1} \end{aligned} \qquad [49]$$

The values $a = 1$, $p = 1$, and $q = \infty$ are obvious. The other limiting values are the interesting ones. They are given by $p = d/(d-1)$, that is, $p = d'$ then $q = 2$ and $a = 2d/(2d-1)$.

These inequalities carry the name of Strichartz inequalities because they are very similar to classical inequalities obtained by Strichartz for the solution of the free Schrödinger equation. This should not be surprising since the Wigner transform of the densities

$$\begin{aligned} f(x,v,t) = \frac{1}{(2\pi)^d} \int & \mathrm{e}^{-\mathrm{i}yv} \psi(x + \tfrac{1}{2}y, t) \\ & \otimes \overline{\psi}(x - \tfrac{1}{2}y, t)\mathrm{d}y \end{aligned} \qquad [50]$$

then turns out to be a solution of the transport equation

$$\partial_t f + v \cdot \nabla_x f = 0 \qquad [51]$$

However, the estimates for kinetic equations are not easily translated into estimations for the Schrödinger equation because the properties of the initial data in terms of norms cannot be simply estimated in terms of the inverse Wigner transform. Spaces with Fourier transform in $L^p, p \neq 2$, are not easy to characterize and not natural for the Schrödinger equation. The above estimates have been very useful in analyzing the large-time behavior of solutions and also in proving the regularity of the three-dimensional Vlasov equation.

The Entropy and Entropy Dissipation

For solutions of the Boltzmann equation the Boltzmann H function

$$H(f) = \int_{\mathbf{R}^3 \times \mathbf{R}^3} f(x,v) \log f(x,v) \mathrm{d}x\, \mathrm{d}v$$

decreases in time and the same is true for the relative entropy to an absolute Maxwellian $M(v) = (2\pi)^{-3/2} \mathrm{e}^{-|v|^2/2}$:

$$H(F|M) = \int_{\mathbf{R}^3 \times \mathbf{R}^3} \left(f \ln\left(\frac{f}{M}\right) - f + M \right) \mathrm{d}x\, \mathrm{d}v$$

This leads to the systematic introduction in the theory of the notion of relative entropy. It turned out to be instrumental in proving relaxation toward equilibrium of solutions of kinetic (or similar) equations and for the analysis of hydrodynamical limits.

A striking example considered by Desvillettes and Villani is the linearized Fokker–Planck equation in any space dimension:

$$\begin{aligned} \partial_t F + v \cdot \nabla_x F - \nabla_x V(x) \cdot \nabla_v F \\ = \nabla_v (\nabla_v F + Fv) \end{aligned} \qquad [52]$$

When $x \mapsto V(x)$ is a smooth potential strictly convex at infinity, this system has a unique steady state given by the relation

$$F_\infty(x,v) = \mathrm{e}^{-V(x)} M(v) = \mathrm{e}^{-V(x)} \frac{\mathrm{e}^{-|v|^2/2}}{(2\pi)^{d/2}} \qquad [53]$$

For any solution of [52] one has

$$\partial_t H(F|M) + \int_{\mathbf{R}^d \times \mathbf{R}^d} F |\nabla_v \log \frac{F}{M}|^2 \,\mathrm{d}x\, \mathrm{d}v = 0 \qquad [54]$$

which says that the entropy dissipation is the relative Fisher information (with respect to v) of F. Now, to study the relaxation to equilibrium, one uses the logarithmic Sobolev inequality:

$$H(F|M) \leq \frac{1}{2} \int_{\mathbf{R}^d \times \mathbf{R}^d} F |\nabla_v \log \frac{F}{M}|^2 \,\mathrm{d}x\, \mathrm{d}v \qquad [55]$$

Details, references, and extensions can be found in Arnold *et al.* (2004).

Conclusions

Kinetic equations have been studied since the end of the nineteenth century, both from the physical and mathematical points of view, but it seems that since the middle of the last century the interest in this approach has considerably increased.

The fact that these equations are well adapted to the description of media which have not "thermalized" (because they are too rarefied or because the domain where they evolve is too small) has been a basic reason for their use in many applied fields; to the ones already quoted one may add the analysis of the air between the reading head and a compact disk, the computations of the characteristics of an ionic motor, and many others.

As a consequence, mathematical progress has been very important. Without going into the details, this contribution is focused on this, and in particular on what can be obtained by the deterministic approach and where the introduction of randomness seems compulsory.

The kinetic formulation turned out to be well adapted to large-scale computers, in particular with Monte Carlo simulations. One should observe that the point of view of modern functional analysis contributes stability estimates to the understanding and improvement of numerical methods. For an introduction to such numerical methods, the reader should first concentrate on the Boltzmann equation itself, which has been one of the basic motivations; consult the book of Sone (2002) the references therein and in particular the book of Bird (1994).

See also: Boltzmann Equation (Classical and Quantum); Breaking Water Waves; Einstein's Equations with Matter; Fourier Law; Interacting Stochastic Particle Systems; Nonequilibrium Statistical Mechanics: Dynamical Systems Approach; Partial Differential Equations: Some Examples; Quantum Dynamical Semigroups.

Further Reading

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Knot Homologies

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Introduction

A knot homology is a theory which assigns to a knot K (or link L) in S^3 a graded homology group whose graded Euler characteristic is a knot polynomial associated to K. In all known examples, the knot polynomials in question are specializations of the HOMFLY polynomial $P_K(a, q)$, which we take to be determined by the skein relation

$$aP(\nwarrow\!\!\!\nearrow) - a^{-1}P(\nearrow\!\!\!\nwarrow) = (q - q^{-1})P(\circlearrowright\circlearrowleft) \qquad [1]$$

and normalized so that P of the unknot is equal to 1. Let $P_N(K)$ be the specialization of P_K given by

$$P_N(K) = P_K(q^N, q) \qquad [2]$$

Then for each $N \geq 0$, there is a bigraded knot homology $H_N^{i,j}(K)$, which satisfies

$$P_N(K) = \sum_{i,j} (-1)^i q^j \dim H_N^{i,j}(K) \qquad [3]$$

We refer to the first grading i as the homological grading, and the second grading j as the polynomial or q-grading.

The idea of a knot homology was introduced by Khovanov (2000) in a seminal paper, in which he defined the homology theory corresponding to the

Jones polynomial ($N=2$). In subsequent work, he defined such a theory for $N=3$, and then, in collaboration with Rozansky, for any $N>0$. Recently, the two authors have introduced a triply graded homology theory $\mathcal{H}^{i,j,k}(K)$ whose graded Euler characteristic gives the entire HOMFLY polynomial:

$$P_K(a,q)=\sum_{i,j,k}(-1)^i q^j a^k \dim \mathcal{H}^{i,j,k}(K) \quad [4]$$

All of these theories are combinatorial in nature.

In contrast, the knot homology for $N=0$ arises from a very different source – the Heegaard Floer homology of Ozsváth and Szabó. This theory traces its roots back to invariants of 3- and 4-manifolds defined using Seiberg–Witten and Donaldson theory. The definition of $H_0(K)$ is not combinatorial, but because of its connections with these invariants, the theory is known to carry a good deal of geometric information about the knot K. The interplay between the two apparently different sorts of knot homologies ($N>0$ and $N=0$) has enhanced our understanding of both sides.

This article will mostly focus on the cases $N=0$ and $N=2$, which are the oldest and best-studied examples of knot homologies and are related to the two best-known specializations of the HOMFLY polynomial – the Alexander and Jones polynomials. We have chosen to use a uniform notation to emphasize the similarities between theories, but the reader should be aware that other notation is more common in the literature. H_0 is often referred to as the knot Floer homology (written *HFK*), and is usually normalized with a polynomial grading of $j'=j/2$, corresponding to the substitution $t=q^2$, which gives the standard normalization of the Alexander polynomial. H_2 is generally called the reduced Khovanov homology, and often denoted by $\mathrm{Kh_r}$ or $\mathrm{Kh_{red}}$.

Construction

Seen from a distance, all knot homologies are defined in much the same way. Given a knot K, we must first choose some additional data D which give a concrete geometric presentation of the knot. Using this data, we write down a bigraded chain complex $(C_N^{i,j}(D), d_N)$. This complex depends on our initial choice of D, but when we take homology, we are left with groups $H_N^{i,j}(K)$ which are invariants of the knot K (cf. the simplicial homology of a topological space X, where the chain groups depend on the choice of some initial geometric data – a triangulation of X – but the homology groups are invariants of X).

In all cases, the generators of $C_N(D)$ correspond naturally to terms which appear in a classical model for computing $P_N(K)$. In other words, we can write

$$P_N(K)=\sum_{\sigma\in S}(-1)^{i(\sigma)}q^{j(\sigma)} \quad [5]$$

where the sum runs over a set of states S determined by D, and the functions i and j are also determined by D. $C_N^{i,j}(D)$ is the free abelian group generated by $\{\sigma\in S|i(\sigma)=i, j(\sigma)=j\}$ and the differential d_N is chosen to preserve the j-grading: $j(d_N x)=j(x)$. It follows that $C_N(D)$ decomposes into an infinite direct sum of complexes, one for each value of j, and [3] is a consequence of [5].

Beyond these global similarities, the definition of $C_N(D)$ varies with the value of N. In the second half of the article, we give explicit details of the constructions for $N=0$ and $N=2$.

Filtered Complexes and Deformations

An important characteristic shared by all the C_N's is the existence of deformations with homology $\mathbb{Z}$. Recall that $(C_N(D), d_N)$ is a graded chain complex: $j(d_N x)=j(x)$. By a deformation of such a complex, we mean a new chain complex $(C_N(D), d_N+d_N')$ in which the underlying group remains the same, but the differential has been perturbed by the addition of a new term d_N' which strictly raises the j-grading: $j(d_N'(x))>j(x)$.

Any deformation of a graded complex is naturally a filtered complex, and as such, gives rise to a spectral sequence. The E_0 term of this spectral sequence is the original unperturbed complex $(C_N(D), d_N)$, so the underlying group of the E_1 term is just $H_N(K)$. Thus, it is independent of the choice of initial data D. In fact, it can often be shown that all terms in the spectral sequence beyond the first one are invariants of K. This is known to be the case for $N=0$ and $N=2$, and is most likely true for all other N as well (cf. the Leray–Serre sequence associated to a fibration, where the first two terms depend on a choice of geometric data but the E_2 and higher terms are all invariants of the fibration).

For each value of N, $C_N(D)$ admits a natural deformation whose homology is $\mathbb{Z}$ in homological grading 0, and zero in every other grading. When $N=0,2$, the filtration grading of this generator is known to be an invariant of K. (This is probably the case for $N>2$ as well.) Equivalently, this is the j-grading of the surviving copy of $\mathbb{Z}$ in the spectral sequence. When $N=0$, this invariant is conventionally normalized to be half the j-grading of the

generator, and is called $\tau(K)$. When $N=2$, it is called $s(K)$.

Geometric Properties

Some elementary properties of the H_N's generalize those of the HOMFLY polynomial. If $K_1 \# K_2$ denotes the connected sum of K_1 and K_2, then over $\mathbb{Q}$

$$H_N(K_1 \# K_2) \cong H_N(K_1) \otimes H_N(K_2) \qquad [6]$$

and if $\bar{K}$ is the mirror image of K,

$$H_N^{i,j}(\bar{K}) \cong H_N^{-i,-j}(K) \qquad [7]$$

Moreover, H_0 satisfies an additional symmetry

$$H_0^{i,j}(K) \cong H_0^{i-j,-j}(K) \qquad [8]$$

generalizing the symmetry of the Alexander polynomial: $P_0(q) = P_0(q^{-1})$. (With integer coefficients, these equalities all hold at the chain level. The correct statements about the homology can be obtained from the Kunneth formula and universal coefficient theorem.)

$H_N(K)$ also contains deeper information related to the genus of surfaces bounding K. If K is a knot in S^3, recall that $g(K)$ – the Seifert genus of K – is the minimal genus of an orientable surface smoothly embedded in S^3 and bounding K. If we view S^3 as the boundary of the 4-ball B^4, we can define a second quantity $g_*(K)$ – the slice genus – by relaxing the requirement that the surface be embedded in S^3 and instead requiring it to be embedded in B^4.

Both $s(K)$ and $\tau(K)$ give lower bounds on the slice genus of K:

$$|\tau(K)| \le g_*(K) \qquad [9]$$

$$|s(K)| \le 2g_*(K) \qquad [10]$$

These bounds are far from independent. In fact, in all known examples, $s(K) = 2\tau(K)$. It is an open problem to determine whether this is true for all knots.

From [6], it follows that s and τ are additive under connected sum. Thus, both invariants define homomorphisms from the concordance group of knots in S^3 to $\mathbb{Z}$. The inequalities in eqns [9] and [10] are not always sharp, but there is one case where equality is known to hold. This is when K is represented by a diagram with all positive crossings (or, more generally, K is quasipositive.) In this case, the slice genus is also equal to the Seifert genus, and all three are easily computed using Seifert's algorithm.

The proof of [10] depends on the fact that for $N > 0, H_N$ is functorial in the following sense. If $S \subset S^3 \times [0,1]$ is a smoothly embedded, orientable cobordism between links L_1 and L_2, then for each $N > 0$, there is an induced map $\phi_N^S : H_N(L_1) \to H_N(L_2)$. ϕ_N^S is a graded map: it preserves the homological grading, and lowers the j-grading by $(N-1)\chi(S)$. Under deformation, it becomes a filtered map which induces a rational isomorphism on the deformed homologies.

H_0 and Heegaard Floer Homology

The proof of [9] depends on the close connection between the knot Floer homology and the Heegaard Floer homology. Roughly speaking, the Heegaard Floer groups of 3-manifolds obtained by surgery on K are determined by the groups $H_0^{i,j}(K)$ together with additional differentials obtained by relaxing the requirement that $n_z(\phi) = n_w(\phi) = 0$. The relation with the slice genus again arises by studying maps induced by cobordisms, but in this case, the relevant cobordism is the surgery cobordism between S^3 and the 0-surgery on K.

This connection also leads to another important property of H_0: it detects the Seifert genus. If we let $M(K)$ be the largest value of j for which the group $H_0^{*,j}(K)$ is nontrivial, then

$$M(K) = 2g(K) \qquad [11]$$

This fact generalizes a well-known inequality involving the degree of the Alexander polynomial: if $m(K)$ is the largest power of q appearing in $P_0(K)$, then $m(K) \le 2g(K)$.

Computations

The difficulty of computing $H_N(K)$ varies with the value of N. When $N=1$, the theory is essentially trivial: $H_1^{0,0}(K) \cong \mathbb{Z}$ for any knot K, and all other groups vanish. Of the remaining knot homologies, $H_2(K)$ is the easiest to compute. The theory for alternating knots was worked out by E S Lee, and extensive calculations have also been made for nonalternating knots using computer programs written by Bar-Natan and Shumakovitch.

Computing H_0 is more difficult, on account of the noncombinatorial nature of d_0. Three families of knots for which H_0 is well understood are alternating knots, (1,1) knots (described in the next section), and knots which admit lens space surgeries. Beyond this, there is an array of techniques which may or may not work in any given case. The best of these is probably a setup introduced by Ozsváth and Szabó, in which the generators of $C_0(D)$ correspond to states in the Kauffman state model of the Alexander polynomial. Combining this method with the known

results for alternating knots and (1,1) knots gives a fairly good understanding of $H_0(K)$ for knots with 10 or fewer crossings; for larger knots, relatively little is known.

Few computations of H_N for $N > 2$ have been made, although the definition in this case is purely combinatorial.

Thin and Thick Knots

For simple knots, both H_0 and H_2 are thin. This means that there exists a constant $c_N(K)(N=0,2)$ such that $H_N^{i,j}(K)$ is trivial unless $j-2i=c_N(K)$. In such cases, we necessarily have $c_0(K)=2\tau(K)$ (resp. $c_2(K)=s(K)$), and $H_N(K)$ is completely determined by $c_N(K)$ and $P_N(K)$. The relationship is best expressed in terms of the Poincaré polynomial of $H_N(K)$:

$$\mathcal{P}_N(K) = \sum_{i,j} t^i q^j \dim H_N^{i,j}(K) = (-t)^{-c_N(K)/2} P_N(K)(q(-t)^{1/2}) \quad [12]$$

If K is an alternating knot, both $H_0(K)$ and $H_2(K)$ are thin, and $c_0(K)=c_2(K)=\sigma(K)$. (Note that in this case the bound on $g_*(K)$ coming from τ and s coincides with the classical bound coming from the signature.) Many nonalternating knots are thin as well; in all examples in which both groups have been computed, either both $H_0(K)$ and $H_2(K)$ are thin, or neither is. In addition, all such knots appear to have $c_0(K)=c_2(K)=\sigma(K)$.

Those knots whose homologies are not thin are called *thick*. There are a dozen such knots with ten or fewer crossings: using the standard numbering in the knot tables (see, e.g., Rolfsen (1976)) these are $8_{19}, 9_{42}, 10_{124}, 10_{128}, 10_{132}, 10_{136}, 10_{139}, 10_{145}, 10_{152}, 10_{153}, 10_{154}$, and 10_{161}. It is a curious and as yet unexplained coincidence that, for all of these knots, the ranks of $H_0(K)$ and $H_2(K)$ are equal.

There is an analogous notion of thinness when $N > 2$, but there exist alternating knots for which H_N cannot be thin for $N \gg 0$ (this can be seen from the HOMFLY polynomials).

Construction of H_0

We now turn to a more detailed description of the definition of $H_0(K)$. The geometric data D used to define C_0 is a Heegaard diagram for the complement of K. One convenient way to specify such a diagram is by a doubly pointed Heegaard diagram of S^3. The data for such a diagram consist of a surface Σ of genus g, two g-tuples of attaching circles $\{\alpha_1, \ldots, \alpha_g\}$ and $\{\beta_1, \ldots, \beta_g\}$ on Σ, and two points $z, w \in \Sigma$ which are disjoint from all the α's and β's. Each set

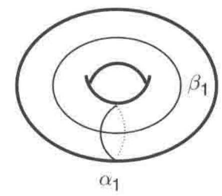


Figure 1 Heegaard splitting of S^3 corresponding to the standard decomposition of S^3 into two solid tori.

of attaching circles is composed of g disjoint simple closed curves, arranged so that when Σ_g is cut along them the result is a sphere with $2g$ holes. Any such set of attaching circles determines a unique genus-g handlebody H with boundary Σ and the property that each attaching circle bounds a disk in H.

The choice of α and β curves determines the underlying 3-manifold in which the knot is embedded. Starting with $\Sigma \times [0,1]$, we fill in one component of the boundary with the handlebody determined by the α-curves, and the other component with the handlebody determined by the β-curves to obtain a closed 3-manifold. By hypothesis, this manifold is required to be S^3. A simple Heegaard diagram of S^3 with $g=1$ is shown in **Figure 1**.

To go from a doubly pointed Heegaard diagram to a diagram of the knot complement, we remove neighborhoods of z and w and replace them with a tube to get a surface Σ' of genus $g+1$. We also add an additional α-handle α_{g+1}, which runs from z to w in Σ in such a way that it does not intersect the other α's, and then comes back over the tube. This process is illustrated in **Figure 2**.

A Heegaard diagram of $S^3 - K$ determines a presentation of $\pi_1(S^3 - K)$ with one generator x_i for each α-circle and one relator w_j for each β-circle. To find the relator w_j, one travels along β_j, recording each intersection with some α_i by appending $x_i^{\pm 1}$ to the relator. The sign is determined by the sign of the intersection. As an example, consider the two doubly pointed diagrams of **Figure 3**, both of which correspond to the same Heegaard diagram of S^3. (It is isotopic to the one shown in **Figure 1**.) The fundamental groups of the associated knot complements can be read off from the corresponding genus-2 Heegaard splittings. Starting from the point where

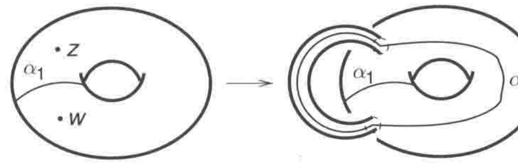


Figure 2 Going from a doubly pointed diagram to a Heegaard diagram of the knot complement.

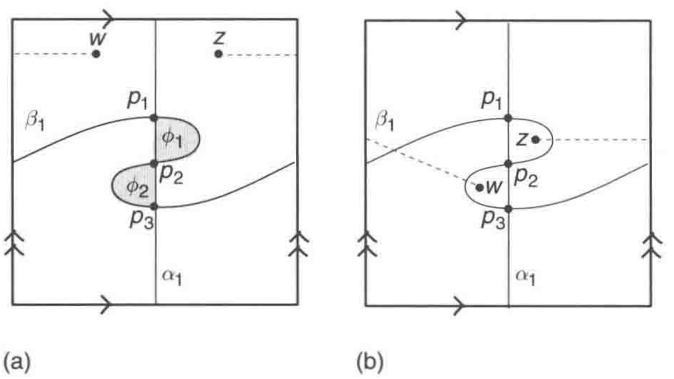


Figure 3 Doubly pointed Heegaard diagrams for the unknot and the trefoil. Opposite sides of the square are identified to form a torus. The dotted line represents α_2.

β_1 intersects the left-hand side of the square and moving to the right, we get

$$\pi_1(S^3 - K_1) = \langle x_1, x_2 | x_1 x_1^{-1} x_1 = 1 \rangle$$
$$\pi_1(S^3 - K_2) = \langle x_1, x_2 | x_2 x_1 x_2^{-1} x_1^{-1} x_2^{-1} x_1 = 1 \rangle$$

The first group is isomorphic to $\mathbb{Z}$, and the knot in **Figure 3a** is the unknot. The second is isomorphic to π_1 of the complement of the trefoil knot, and in fact the knot in **Figure 3b** is the left-handed trefoil.

The definition of $C_0(D)$ is based on a classical method for computing the Alexander polynomial known as the Fox calculus, which takes as its input a presentation of $\pi_1(S^3 - K)$. According to Fox calculus,

$$P_0(K) = \pm q^n \det(d_{x_i} w_j)_{1 \le i,j \le g} \qquad [13]$$

Here $d_{x_i} w_j$ is an element of the group ring

$$\mathbb{Z}[H_1(S^3 - K)] \cong \mathbb{Z}[q^{\pm 2}]$$

It is determined by the following rules:

$$d_{x_i} x_j = \delta_{ij} \qquad [14]$$

$$d_{x_i} ab = d_{x_i} a + |a| d_{x_i} b \qquad [15]$$

$$d_{x_i} x_i^{-1} = -|x_i^{-1}| \qquad [16]$$

where

$$|\cdot| : \pi_1(S^3 - K) \to H_1(S^3 - K) \cong \mathbb{Z} = \langle q^2 \rangle \qquad [17]$$

is the abelianization map. The factor of $\pm q^n$ is chosen so that $P_0(K)(1) = 1$ and $P_0(K)(q) = P_0(K)\ (q^{-1})$.

As an example, consider the two presentations above. In the first presentation, $|\cdot|$ sends x_1 to 1 and x_2 to q^2, so

$$d_{x_1}(x_1 x_1^{-1} x_1) = 1 - |x_1 x_1^{-1}| + |x_1 x_1^{-1}|$$
$$= 1 - 1 + 1$$
$$= 1 \qquad [18]$$

which is the Alexander polynomial of the unknot. If we abelianize the relator in the second presentation, we see that $|x_1| = |x_2| = q^2$, so

$$d_{x_1}(x_2 x_1 x_2^{-1} x_1^{-1} x_2^{-1} x_1)$$
$$= |x_2| - |x_2 x_1 x_2^{-1} x_1^{-1}| + |x_2 x_1 x_2^{-1} x_1^{-1} x_2^{-1}| \qquad [19]$$
$$= q^2 - 1 + q^{-2} \qquad [20]$$

which is the Alexander polynomial of the trefoil.

When $g = 1$, the complex $C_0(D)$ is generated by the points of $\alpha_1 \cap \beta_1$. These intersection points may be naturally identified with the appearances of the generator x_1 in w_1, and thus with the monomials appearing in $d_{x_1} w_1$. For example, the three monomials which appear on the right-hand sides of eqns [18] and [19] correspond, respectively, to the points labeled p_1, p_2, and p_3 in **Figure 3**. The j-grading of each generator is given by the exponent of q which the corresponding monomial contributes to the Alexander polynomial. Thus, all three generators in **Figure 3a** have j-grading 0, while in **Figure 3b**, the generators p_1, p_2, and p_3 have j-gradings 2, 0, and –2 respectively.

For general g, the monomials appearing in the determinant of eqn [13] correspond to intersection points of the two totally real tori $\alpha = \alpha_1 \times \cdots \times \alpha_g$ and $\beta = \beta_1 \times \cdots \times \beta_g$ inside the symmetric product $\mathrm{Sym}^g \Sigma$. The knot Floer homology is the Lagrangian Floer homology of α and β inside the symplectic manifold $\mathrm{Sym}^g(\Sigma - z - w)$. The generators of $C_0(D)$ are the points of $\alpha \cap \beta$; the differential is defined by counting holomorphic disks with boundary on α and β. To be precise, for $x \in \alpha \cap \beta$,

$$d_0 x = \sum_{\substack{\phi \in \pi_2(x,y), \mu(\phi)=1 \\ n_z(\phi) = n_w(\phi) = 0}} \# \mathcal{M}(\phi) y \qquad [21]$$

Here $\pi_2(x, y)$ denotes the set of homotopy classes of maps of the strip $D = \{a + ib \mid b \in [0,1]\}$ into $\mathrm{Sym}^g \Sigma$ which take the right-hand boundary to α and the left-hand boundary to β, and which limit to x as $b \to -\infty$ and to y as $b \to \infty$. $\mu(\phi)$ denotes the formal dimension of the space of pseudoholomorphic disks in this homotopy class. There is a natural action by translation on the space of such maps, so when $\mu(\phi) = 1$ we can divide out by this action and obtain an oriented zero-dimensional moduli space $\mathcal{M}(\phi)$. Finally, by $n_z(\phi)$ and $n_w(\phi)$ we denote the intersection number of such a strip with the divisors determined by z and w inside of $\mathrm{Sym}^g \Sigma$. The requirement that they vanish forces the strip to lie

in $\mathrm{Sym}^g(\Sigma - z - w)$. It can be shown that, for $\phi \in \pi_2(x, y)$,

$$j(x) - j(y) = n_z(\phi) - n_w(\phi) \qquad [22]$$

so $j(d_0 x) = j(x)$.

When $g = 1$, computing the differential amounts to counting maps of the strip into the Heegaard torus. This can be done algorithmically using the Riemann mapping theorem, so computation of H_0 is purely combinatorial. Knots of this form are called (1,1) knots. They are one of our few windows into the behavior of H_0 for large knots.

As an example, consider the diagram of **Figure 3a**. The two shaded regions represent the domains of classes $\phi_1 \in \pi_2(p_1, p_2)$ and $\phi_3 \in \pi_2(p_3, p_2)$. The Riemann mapping theorem implies that up to reparametrization, there is a unique holomorphic map of the strip into each region, so $\#\mathcal{M}(\phi_1) = \pm 1 = \#\mathcal{M}(\phi_2)$. The differential in $C_0(D_1)$ is given by

$$d_0(p_1) = \pm p_2 = d_0(p_3)$$
$$d_0(p_2) = 0$$

and $H_0(U) \cong \mathbb{Z}$. This reflects the fact that we could have chosen the more efficient diagram of $S^3 - U$ shown in **Figure 1**, simply by moving β_1 to remove two of the intersection points.

For comparison, consider the diagram for the trefoil shown in **Figure 3b**. All three generators of $C_0(D_2)$ have different j-gradings, so we must have $d_0 \equiv 0$. Thus, $H_0(T) \cong \mathbb{Z}^3$. The two disks ϕ_1 and ϕ_2 are still present, but now $n_z(\phi_1) = n_w(\phi_2) = 1$, so neither disk contributes to the differential. This is reflected in the fact that β_1 cannot be moved to reduce the number of intersection points without passing through either z or w.

Deformations

In this case, finding an appropriate deformation of $C_0(D)$ is simple: we just drop the condition that $n_z(\phi) = 0$ in the definition of the differential. If a homotopy class $\phi \in \pi_2(x, y)$ contributes nontrivially to the sum, it must have a holomorphic representative, which necessarily intersects the divisor in $\mathrm{Sym}^g\Sigma$ defined by z non-negatively. Thus, $n_z(\phi) \geq 0$. From [22], it follows that $j(x) - j(y) = n_z(\phi) \geq 0$, so this new differential has the form $d_0 + d_0'$, where d_0' strictly lowers the j-grading.

The fact that the homology of $C_0(D)$ with respect to the perturbed differential is $\mathbb{Z}$ goes back to the knot Floer homology's roots in Heegaard Floer homology. By dropping the condition that $n_z(\phi) = 0$, we have effectively forgotten about the basepoint z, and thus about the knot. The new complex simply computes the Heegaard Floer group $\widehat{HF}(S^3)$, which is isomorphic to $\mathbb{Z}$. When $g = 1$, this can be seen directly: if we remove the basepoint z, any genus-1 Heegaard diagram of S^3 can be isotoped into the standard diagram of **Figure 1**.

Construction of H_2

In this case, the geometric data D needed to define the chain complex $C_2(D)$ is a planar diagram of the knot, and the classical model on which the construction of $C_2(D)$ is based is the Kauffman state model for the Jones polynomial. There is a related homology theory $\tilde{H}_2(D)$, known as the unreduced Khovanov homology, whose graded Euler characteristic is $(q + q^{-1})P_2(K)$. This is the original categorification of the Jones polynomial defined in Khovanov (2000).

To construct $\tilde{C}_2(D)$, we consider complete resolutions of the planar diagram D. As shown in **Figure 4**, there are two different ways to resolve each crossing of D. If D has n crossings, there will be 2^n ways to resolve all n, one for each vertex of the cube $[0, 1]^n$. To a vertex v, we associate the crossingless planar diagram D_v obtained from the corresponding resolution of D. Thus, each vertex of the cube is decorated by a 1-manifold D_v.

If e is an edge joining vertices v_0 and v_1 (where v_0 has one more 0 coordinate than v_1), we write $e: v_0 \to v_1$, and decorate e with a two-dimensional cobordism S_e from D_{v_0} to D_{v_1}. S_e is a product cobordism outside a neighborhood of a single crossing, where it is the one-handle cobordism between the 0-resolution and the 1-resolution. The resulting cobordism is necessarily composed of a union of product cobordisms (cylinders) together with a single nontrivial cobordism (a pair of pants). Thus, starting from D, we have constructed an n-dimensional cube whose vertices are decorated by 1-manifolds and whose edges are decorated by cobordisms between them. This is the cube of resolutions of D.

The next step in the construction of $\tilde{C}_2(D)$ is to apply a graded $(1 + 1)$-dimensional TQFT $\mathcal{A}$ to the cube of resolutions. $\mathcal{A}$ is a functor which associates to each 1-manifold X a group $\mathcal{A}(X)$, and to each two-dimensional cobordism $W: X_1 \to X_2$ a homomorphism $\mathcal{A}(W): \mathcal{A}(X_1) \to \mathcal{A}(X_2)$. If we apply $\mathcal{A}$ to all the manifolds and cobordisms of the cube of

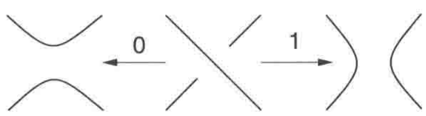


Figure 4 0- and 1-resolutions of a crossing.

Table 1 Summary of cube of resolutions

Vertex v	$\rightarrow$	1-manifold D_v	$\rightarrow$	Group $\mathcal{A}(D_v)$
Edge $e: v_1 \rightarrow v_2$	$\rightarrow$	Cobordism $S_e: D_{v_1} \rightarrow D_{v_2}$	$\rightarrow$	Homomorphism $\mathcal{A}(S_e): \mathcal{A}(D_{v_1}) \rightarrow \mathcal{A}(D_{v_2})$

resolutions, we obtain a new cube, decorated with groups and cobordisms between them. This process is summarized in **Table 1**.

We can now describe the chain complex $\tilde{C}_2(D)$. As a group,

$$\tilde{C}_2(D) = \bigoplus_v \mathcal{A}(D_v) \quad [23]$$

where the sum runs over all vertices of the cube of resolutions. For $x \in \mathcal{A}(D_v)$, the differential is given by

$$d_2 x = \sum_{e: v \rightarrow v'} (-1)^{s(e)} \mathcal{A}(S_e)(x) \quad [24]$$

The signs in this sum are determined by assigning a sign $(-1)^{s(e)}$ to each edge e in such a way that every two-dimensional face of the cube has an odd number of $-$ signs on its edges. (This ensures that $d^2 = 0$.) There are many ways to do this, but they all result in isomorphic complexes.

The homological grading i on $\tilde{C}_2(D)$ is easily determined. For $x \in \mathcal{A}(D_v)$, we set $i(x) = i(v) - c(D)$, where $i(v)$ is the sum of all the coordinates of v, and $c(D)$ is a constant. Clearly, $i(d_2 x) = i(x) + 1$. In order to have invariance, it turns out that $c(D)$ must be chosen to be equal to the number of negative crossings in D.

It remains to specify the TQFT $\mathcal{A}$. At the level of groups, $\mathcal{A}(S^1)$ is a free abelian group of rank 2:

$$\mathcal{A}(S^1) = A = \langle 1, X \rangle \quad [25]$$

General principles then imply that

$$\mathcal{A}\Big(\coprod^n S^1\Big) = A^{\otimes n} \quad [26]$$

To specify the maps induced by cobordisms, it is enough to describe the maps associated to the two pairs of pants shown in **Figure 5**. They are given by

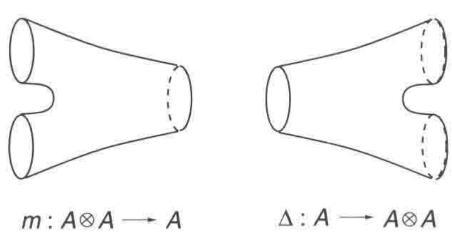


Figure 5 Maps induced by pairs of pants.

$$m(1 \otimes 1) = 1$$
$$\Delta(1) = 1 \otimes X + X \otimes 1 \quad [27]$$

$$m(1 \otimes X) = m(X \otimes 1) = X$$
$$\Delta(X) = X \otimes X \quad [28]$$

$$m(X \otimes X) = 0 \quad [29]$$

Note that the multiplication m makes A into a commutative ring isomorphic to $\mathbb{Z}[X]/(X^2)$.

$\mathcal{A}$ is a graded TQFT. In other words, there is a grading q on A and its tensor products, determined by

$$q(1) = 1$$
$$q(a \otimes b) = q(a) + q(b) \quad [30]$$

$$q(X) = -1 \quad [31]$$

From eqns [27]–[29], it is easy to see that

$$q(m(a \otimes b)) = q(a \otimes b) - 1$$
$$q(\Delta(a)) = q(a) - 1 \quad [32]$$

If we define $j(x) = k(D) + q(x) + i(x)$, it follows that $j(d_2 x) = j(x)$. Taking the graded Euler characteristic gives

$$\chi(\tilde{C}_2(D)) = q^{k(D)} \sum_v (-q)^{i(v)} (q + q^{-1})^{n_v} \quad [33]$$

where n_v is the number of components of D_v. If we define $k(D)$ to be the writhe of D, this is precisely Kauffman's formula for the unnormalized Jones polynomial.

Figure 6 illustrates $\tilde{C}_2(D)$ for a simple two-crossing link. The figure shows the original link (in the center), the cube of resolutions, and basis vectors for $\tilde{C}_2(D)$, together with their j-gradings. We leave it to the reader to check that the homology $\tilde{H}_2(L)$ is four dimensional, supported in j-gradings 1 and 3 at the vertex labeled 00, and in gradings 5 and 7 at the vertex labeled 11.

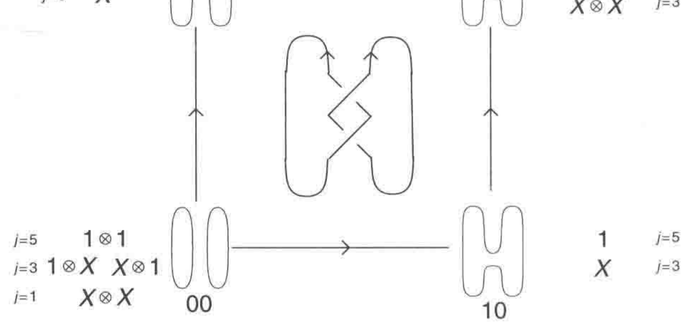


Figure 6 The cube of resolutions for the Hopf link.

To get the reduced chain complex $C_2(D)$, we must divide the graded Euler characteristic by a factor of $(q+q^{-1})$. This is accomplished by choosing a marked point on K and requiring that for each resolution D_v, the vector associated to the circle containing the marked point lie in the subspace of A spanned by X. If D is a diagram of a knot, the resulting homology $H_2(K)$ is independent of the choice of marked point. For links, $H_2(L)$ depends on the component of the link on which the marked point lies.

Deformations

Deformations in the $N=2$ theory are constructed using a technique introduced by E S Lee. The idea is to replace the graded TQFT $\mathcal{A}$ with a filtered TQFT $\mathcal{A}'$. As a group, we still have $\mathcal{A}(S^1)=A$, but the multiplication and comultiplication maps are perturbations of those for $\mathcal{A}$:

$$m'(1\otimes 1)=1 \qquad \Delta'(1)=1\otimes X+X\otimes 1-r1\otimes 1 \qquad [34]$$

$$m'(1\otimes X)=m'(X\otimes 1)=X \qquad \Delta'(X)=X\otimes X+s1\otimes 1 \qquad [35]$$

$$m'(X\otimes X)=rX+s \qquad [36]$$

The new terms involving r and s have q gradings strictly greater than the terms which are shared with eqns [27]–[29]. Thus, the differential defined by replacing m and Δ by m' and Δ' will be a perturbation of the original differential on $\tilde{C}_2(D)$.

The simplicity of the homology with respect to the new differential depends on the fact that when the polynomial X^2-rX-s has simple roots, the TQFT $\mathcal{A}'$ decomposes as a direct sum of two one-dimensional TQFTs. This implies that for a knot, the deformed homology $\tilde{H}'_2(K)$ decomposes as a direct sum of two copies of $H_1(K)$. This group is always isomorphic to $\mathbb{Z}$, so $\tilde{H}'_2(K)\cong\mathbb{Z}\oplus\mathbb{Z}$. If $s=0$, the same strategy can be used to define deformations of the reduced chain complex $C_2(D)$. In this case, we find that the deformed homology is isomorphic to a single copy of $\mathbb{Z}$.

See also: Floer Homology; Gauge Theory: Mathematical Applications; The Jones Polynomial; Knot Theory and Physics; Topological Quantum Field Theory: Overview.

Further Reading

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Knot Invariants and Quantum Gravity

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Introduction

As in all other physical theories, one expects that gravitational phenomena will ultimately be ruled by quantum mechanics. This requires to consider the quantization of the best available theory of gravity, namely Einstein's general relativity. This problem has been considered since the 1930s (*see* Loop Quantum Gravity). The application of the rules of quantum mechanics to general relativity is immediately problematic. Unlike other physical interactions, general relativity describes gravitational phenomena through a distortion of spacetime rather than through a field living in spacetime. Therefore, its quantization is bound to be very different from that of other physical theories. In particular, the well-established framework of perturbative quantum field theory, used with remarkable success in describing electroweak and strong interactions (in the latter case at least in certain regimes), runs into trouble when applied to general relativity. At present, it is not clear if this is a fundamental problem or if there might exist an implementation of perturbative quantum field theory that works well in the gravitational case. On the

other hand, there exist examples of field theories where perturbative methods fail but that nevertheless can be quantized. This suggests that the consideration of nonperturbative techniques in the quantization of the gravitational field could be a promising avenue.

In particular, canonical quantization methods appear attractive for attempting a nonperturbative quantization of gravity. Canonical methods force the introduction, in a clear way, of a Hilbert space of states and definition of the quantum operators of interest. The application of canonical methods to classical general relativity was pioneered by Dirac and Bergmann in the late 1950s. During the 1960s, the resulting canonical theories were considered in a quantum setting by DeWitt. At the time it appeared that making progress in the canonical quantization of general relativity was going to be quite a challenge. In particular, the canonical theory has constraints, which have to be implemented as operator identities quantum mechanically. The wave functions were functionals of the spatial metric of spacetime. One of the operator identities to be satisfied implies that the wave functions only depend on properties of the spatial metric that are invariant under spatial diffeomorphisms. This is a direct consequence of general relativity being a theory that is independent of coordinate choice since a diffeomorphism changes the assignment of coordinates to points in the manifold. Finding such wave functions already presented a challenge, since there is no well-grounded mathematical theory of functionals of diffeomorphism-invariant classes of metrics. Moreover, the other operator identity to be imposed, known as the Hamiltonian constraint or Wheeler–DeWitt equation, was a nonpolynomial complicated operator equation that does not admit a simple geometrical interpretation and needs to be regularized. Since one does not have a background metric to rely upon, traditional regularization techniques of quantum field theory are not suitable to deal with the Hamiltonian constraint.

These difficulties severely hampered development of canonical methods for the quantization of general relativity for approximately two decades. The situation started to change when Ashtekar noticed that one could choose a different set of variables to describe general relativity canonically. Instead of using as variable the spatial metric q_{ab}, Ashtekar chooses to use a set of (densitized) frame fields $\tilde{E}^a_i$. The relationship between the metric and the densitized frames is $\det(q^{ab})q^{ab} = \tilde{E}^a_i\tilde{E}^b_i$ and we are assuming the Einstein summation convention, that is, the index i is summed from 1 to 3 (such an index labels which vector in the triad one is referring to). The resulting theory has an additional symmetry with respect to usual general relativity, in the sense that it is invariant under the choice of frame. This symmetry operates on the index i as if it were an SO(3) symmetry. As canonical momenta the usual choice is to pick the extrinsic curvature of the 3-geometry. Ashtekar chooses a variable related to it that behaves under frame transformations as an SO(3) connection, A^i_a. The resulting theory is therefore cast in terms of a canonical pair $(\tilde{E}^a_i, A^i_a)$, with i an SO(3) index. One can therefore consider the canonical pair as that of a Yang–Mills theory associated with the SO(3) group. In fact, associated with the extra symmetry under triad rotations the theory has a new set of constraints that take the form of a Gauss law, $D_a\tilde{E}^a_i = 0$ with D_a the covariant derivative formed with the connection A^i_a. This allows us to view the phase space of a Yang–Mills theory as the kinematical arena on which to discuss quantum gravity. The theory is of course different from the Yang–Mills theory. In particular, it still has constraints that imply that it is invariant under spacetime diffeomorphisms. In the canonical picture, these constraints appear asymmetrically as one constraint is associated with time evolution ("Hamiltonian constraint") and a set of three constraints is associated with spatial diffeomorphisms ("diffeomorphism constraint").

If one quantizes the theory starting from the Ashtekar formulation, given the resemblance with Yang–Mills theory, the natural choice for a representation of the quantum wave functions is to consider wave functions of the connection $\Psi[A]$ that are invariant under SO(3) transformations. Such a representation is known as "connection representation." There is significant experience in Yang–Mills theory in constructing such wave functions. In particular, it is known that if one considers the parallel transport operator defined by a connection around a closed curve (holonomy) and one takes its trace ("Wilson loop"), the resulting object is invariant under SO(3) transformations. What is more important, the set of traces of holonomies along all possible closed loops is an overcomplete basis for all gauge-invariant functions. More recently, it has been shown that one can construct a less redundant complete basis using techniques from spin networks. We will discuss later on how to do this.

Since any gauge-invariant functional can be expanded in the basis of Wilson loops, one can choose to represent it through the coefficients of such an expansion. These coefficients are functions of the curve upon which the corresponding element of the basis of Wilson loops is based. The representation of wave functions in terms of such coefficients is called "loop representation." Wave

functions in the loop representation are functions of a closed curve (more precisely of families of closed curves, or spin networks, as we will discuss below).

We still have to deal with the diffeomorphism and Hamiltonian constraints. The diffeomorphism constraint when written in the loop representation implies that the wave functions are not functions of loops but rather of topologically invariant properties of the loops under general diffeomorphisms of the spatial manifold containing the loops. Such functions are technically known in the mathematical literature as "knot invariants." This is the first point of connection between knot invariants and quantum gravity; they constitute the kinematical arena of the theory. One still has to deal with the Hamiltonian constraint, which has to be imposed as an operator equation. We shall see that knot theory also seems to have a lot to say about solutions of the Hamiltonian constraint. This is quite remarkable, since the Hamiltonian constraint embodies in detail the specific dynamics of Einstein's theory of gravitation, and to our knowledge this is an input that has never gone into the ideas of knot theory.

In terms of the Ashtekar variables, the Hamiltonian constraint takes the form

$$H = \boldsymbol{E}^a \cdot \boldsymbol{E}^b \times (\boldsymbol{B}^c + \Lambda \boldsymbol{E}^c)\epsilon_{abc} \qquad [1]$$

where we have used a conventional vector notation for the frame indices and kept explicit the spatial indices. ϵ_{abc} is the Levi-Civita totally antisymmetric tensor. We have included a possible cosmological constant Λ. The Ashtekar formulation can be constructed in different ways. In the original formulation, the connection A_a^i was a complex variable and the Hamiltonian took the form we listed above. However, the resulting theory was only equivalent to real general relativity if the variables satisfied certain reality conditions. One can choose to use a real connection instead, but then the Hamiltonian constraint has additional terms. At the moment, we will concentrate on the constraint as listed above. The constraint has to be implemented as a quantum operator acting on wave functions. Since it involves the product of operators, it needs to be regularized. Most regularization methods are problematic in this context, since they use a metric, and here the metric is a quantum operator, not an external fixed quantity. If we ignore these difficulties, one observes that, if one were to choose a quantum state, for instance in the connection representation, for which,

$$\Lambda \hat{E}_i^a \Psi[A] = -\hat{B}_i^a \Psi[A] \qquad [2]$$

the state would be annihilated by the Hamiltonian constraint, and this would be true no matter what regularization was chosen. Classically, the condition $E_i^a \sim B_i^a$ is satisfied for the de Sitter geometry, so one could envision the state as a quantum state associated with such geometry. The exact solution of the above equation is given by a state that is the exponential of the integral on the spatial slice of the Chern–Simons form built from the connection

$$\Psi_{\mathrm{CS}}[A] = \exp\left(k \int \mathrm{d}^3x \, \mathrm{tr}(A \wedge dA + \frac{2}{3} A \wedge A \wedge A)\right) \qquad [3]$$

and the constant k needs to be chosen as $k = 6/\Lambda$ for the state to be a solution.

One can ask, "what is the expression of this state in the loop representation?" To answer this, one needs to compute the coefficients of its expansion in the basis of Wilson loops $W_\gamma[A]$, where as we stated earlier, γ should be a collection of (intersecting) loops (later we will discuss the generalization to spin networks). The expression for the coefficients will be a function only of the loops γ and is given by

$$\Psi_{\mathrm{CS}}[\gamma] = \int DA \, W_\gamma[A] \Psi_{\mathrm{CS}}[A] \qquad [4]$$

This expression is invariant under diffeomorphisms of the manifold or, equivalently, under smooth deformations of the curve γ. That is, it is what in the mathematical literature is called "knot invariant." In fact, this integral has been studied by Witten in the context of Chern–Simons theory and has been shown to be related to the Kauffman bracket knot polynomial, which in turn is related to the celebrated Jones polynomial. Therefore, the implication of these results is that the Kauffman bracket knot polynomial appears to be the representation in the loop representation of a state of quantum gravity that solves the quantum Einstein equations (with a cosmological constant). The reader may be intrigued by the word "polynomial" in this context. It should be noted that the Chern–Simons state $\Psi_{\mathrm{CS}}[A]$ depended on a parameter k, which had to take a certain value for it to solve the quantum Einstein equations. The resulting knot invariant is a polynomial in $\exp(k)$. If one expands out the result, an infinite power series in k results. There will be infinite coefficients in the series, but they are just combination of the finite number of coefficients of the polynomial. Knot polynomials are a powerful tool for analyzing and distinguishing knots. The coefficients of the polynomials are all knot invariants. Typically, for "simple" knots, the first few coefficients of the knot polynomial are nonzero. As one considers more complicated knottings, higher

coefficients become nonvanishing. The ultimate goal of knot theory is to be able to consider two arbitrary knots and to unambiguously determine if the two knots are related by a smooth transformation. The knot polynomials appear as promising tools for achieving this task that has remained elusive up to now.

Returning to quantum gravity, to have a well-known knot polynomial as a solution of the quantum Einstein equations is a remarkable fact. The first connection we outlined between knot theory and quantum gravity was less unexpected: if one describes a theory that is diffeomorphism invariant in terms of loops, the appearance of knots is inevitable. But we are now finding that knot invariants from the mathematical literature, which were constructed without any knowledge of the details of the dynamics of the Einstein equations, seem to manage to solve such equations. This is either a big coincidence or a pointer to some unexplained deep connection yet to be understood. Notice, for instance, that other theories of gravity would not have the Kauffman bracket as a quantum state.

There is a certain technicality about the Kauffman bracket that makes it difficult to argue with precision that it is a state of quantum gravity. To understand this technicality better, it is perhaps best to concentrate on the form of the quantum state written above if the connection is an abelian connection. In that case, the integral in question,

$$\Psi_{\text{CS abelian}}[\gamma] = \int DA \oint_\gamma \mathrm{d}y^a \exp(\mathrm{i}A_a) \times \exp\left(\int \mathrm{d}^3x \epsilon^{abc} A_a \partial_b A_c\right) \quad [5]$$

by turning it into a Gaussian integral. The result is

$$\Psi_{\text{CS abelian}}[\gamma] = \oint_\gamma \mathrm{d}x^a \oint_\gamma \mathrm{d}y^b \epsilon_{abc} \frac{(x-y)^c}{|x-y|} \quad [6]$$

This integral has problems, since the integrand is ill-defined when $x = y$. Notice that the integral would be well defined if the two contour integrals were evaluated on different, nonintersecting curves. The result would be the well-known formula for the Gauss linking number of the curves, yielding zero if they are not linked and and integer multiple of 4π if they were. So the integral we were trying to compute was actually the Gauss linking number of the curve with itself. Such a quantity is not well defined for ordinary curves. To deal with this problem, mathematicians introduced the concept of framed knots. A framed knot is a curve with a prescription to determine a second curve from it. One way to see it is to construct another curve that is "infinitesimally close" in space to the original one. It is clear that there is no canonical way to compute such a second curve. Then, when one considers quantities like the self-linking number, one makes them well defined by evaluating the two integrals on the two curves, the original one and the one yielded by the prescription. In reality, the notion of framing is a bit more elaborate than what we hint at here, since one could consider invariants constructed with more than two integrals and could still be ill-defined if one only considers two curves. The notion has to be extended as well to handle intersections in the curves. We will ignore these subtleties in this discussion.

The Kauffman bracket knot invariant is an invariant of framed knots, just like the self-linking number. It is not well defined for a single curve. It requires a framing of the knot. In quantum gravity, there is no compelling reason to consider framed curves. It is true that framed curves arise naturally in q-deformed field theories and perhaps a q-deformed version of quantum gravity is what needs to be considered to accommodate the Chern–Simons state, but at the moment there are no proposals along these lines that have widespread consensus.

So, it appears the Kauffman bracket does not have a natural role to play as a state of quantum gravity. However, it is known that the frame dependence of the Kauffman bracket knot polynomial can be captured in an overall factor that depends on the self-linking number. If one strips the polynomial of this factor, one gets the Jones polynomial, which is a knot invariant of single curves. Could it be that this polynomial has a chance of being a solution of the quantum Einstein equations?

To determine this, the analogy with Chern–Simons theory is no longer useful, since there is no straightforward way to transform the relation between the Kauffman and Jones polynomials into relations between states in the connection representation. To analyze if the Jones polynomial could be a solution of the quantum Einstein equations, one needs to write the quantum Einstein equations directly in terms of loops.

There have been several attempts to rewrite the quantum Einstein equations directly in the loop representation. In one of these attempts, the curvature that appears in the Hamiltonian constraint was represented by the "loop derivative." This is a differential operator that can be introduced in the space of loops by considering that two loops that differ by a small element of area are "close." One can build an attractive differential calculus in loop space that actually encodes many of the kinematical properties that are useful to formulate Yang–Mills theory.

The Hamiltonian constraint in terms of the loop derivative is an operator that has an explicit form. The coefficients of the Jones polynomial can also be given an explicit form by computing perturbatively the integral in the Chern–Simons theory. The results are generalizations of the types of integrals that arise in the self-linking number, but involving a larger number of integrals. One can therefore envisage carrying out an explicit computation in which one checks if the coefficients of the Jones polynomial are annihilated or not by the Hamiltonian constraint of quantum gravity in the loop representation. Such a calculation has been carried out for the first few coefficients. It turns out that the second coefficient (the first coefficient is normalized to unity, so it trivially satisfies the constraint) is indeed annihilated by the Hamiltonian constraint of vacuum quantum gravity (with zero cosmological constant). It has been shown that the third coefficient is not, and there are good arguments to indicate that other coefficients will not be states of quantum gravity.

So, a remarkable result has been found in that one of the coefficients of the Jones polynomial (related to the Arf and Casson invariants) is annihilated by a version of the quantum Hamiltonian constraint of general relativity. The result is quite nontrivial; it requires a fair amount of calculation to actually show that the coefficient is annihilated. The meaning of this quantum state and the deep reason why it is annihilated remain at present a mystery.

The quantum Hamiltonian constraint based on the loop derivative makes certain assumptions about the space of functions one is using to quantize the theory. In quantum field theory, not all classical operators have a well-defined quantum counterpart. The choice being made is to assume that the curvature F_{ab} is a well-defined quantum operator defined by the loop derivative. Differentiability of knot polynomials is not a new idea. It is the core idea of the Vassiliev knot invariants, which are defined by a set of identities, one of them acting as a "derivative in knot space." It can be shown that the loop derivative is a concrete implementation of the Vassiliev derivative and, therefore, Vassiliev invariants are the "arena" in which this version of quantum gravity takes place.

The Hamiltonian based on the loop derivative has problems, in the sense that it is obtained by a regularization procedure that requires extra external geometric structures. This is common practice in Yang–Mills theory, where one has at hand a fixed external background metric. However, in gravity the geometry is a dynamical object and, if one constructs expressions that resort to some fixed external geometry, one gets inconsistencies. In particular, it is expected that the Hamiltonian based on the loop derivative will not reproduce the correct Poisson algebra of canonical general relativity. This sort of problem plagued early attempts to construct a quantum version of the Hamiltonian constraint in the early 1990s.

A point that we mentioned earlier but did not elaborate upon, is that the Wilson loops constitute an overcomplete basis of states. Therefore, if one takes a quantum state and expands it on such a basis, one gets that the coefficients of the expansion satisfy certain identities, called the Mandelstam identities. These are nonlinear identities that states in the loop representation have to satisfy. These identities are very inconvenient at the time of constructing quantum states. The identities stem from the fact that if one chooses a matrix representation of the group of interest, the fact that one is in a given representation is indicated by certain identities the matrices satisfy. To break free from these constraints, one possibility is to consider multiple representations when constructing Wilson loops. To do this, one considers piecewise-continuous graphs with intersections (the nonintersecting case is a trivial subcase). Along the lines connecting the intersections one considers holonomies in a given representation for a given line. In the case of the group SU(2), which is the one of interest in quantum gravity, such representations are labeled by a (half-) integer. One then considers invariant tensors in the group to "tie the holonomies together" at intersections. The resulting object is a gauge-invariant object for a given connection based on a "spin network." The latter is an embedded piecewise-continuous graph with an assignment of integers to each of its lines and an assignment of "intertwiners" at each intersection (if the intersections are trivalent or lower, one can choose canonical intertwiners and forget about them).

One can then consider the "spin network representation" in which one expands gauge-invariant states in terms of the basis of Wilson nets. Knot polynomials for these types of graphs have been considered in the mathematical literature ("polynomials of colored graphs"). The construction with the Chern–Simons state can be repeated, and there exist suitable generalizations of the Kauffman bracket and Jones polynomials. The Hamiltonian based on the loop derivative can also be introduced in this context; again, its action is well defined on suitable generalizations of Vassiliev invariants for these kinds of graphs. This opens the possibility of encoding the quantum dynamics of general relativity as a combinatorial action in the space of Vassiliev invariants.

An alternative Hamiltonian based on assuming that the holonomies and the volume operators are well defined quantum mechanically (but not the curvature) has been introduced that has the advantage of not

requiring external structures for its regularization. In fact, it can be explicitly checked that it satisfies the correct Poisson algebra without anomalies at the quantum level. The exploration of the action of this Hamiltonian constraint on knot polynomials has not been carried out as systematically as for the one based on the loop derivative, but it has been explicitly shown that the first coefficient in the expansion of the Jones polynomial is annihilated by this Hamiltonian constraint. The first coefficient, written in terms of loops, was simply the numeral 1 and was automatically annihilated. In terms of spin network states, the first coefficient is the "chromatic evaluation" of the network (the result of computing the Wilson loop on a connection that is pure gauge). It is somewhat nontrivial to show that this quantity is actually annihilated by the Hamiltonian constraint in question.

At the moment, the issue of what the correct Hamiltonian constraint is that describes a realistic and physically correct theory of quantum gravity is still open to debate. There are certain concerns that the action of the operators considered up to now is too simple to encompass the true dynamics of general relativity. Constructing a semiclassical theory that could confirm or deny the viability of the proposals is a complicated task, since one has to make contact with physics that is not diffeomorphism invariant in the context of a theory that is. Moreover, in canonical quantum gravity, there exists the "problem of time." Since the Hamiltonian vanishes, the dynamics implied by it is trivial, and one has to disentangle the true dynamics by relational constructions among the variables of the theory. One then needs to compare the resulting predictions with classical general relativity.

Whether the current proposals are viable and whether knot theory will play a role at a "kinematical level" or it will actually play a key role in the detailed dynamics of quantum general relativity is yet to be seen. It is reassuring that in partial constructions, celebrated knot polynomials have appeared to have some knowledge of the dynamics of the Einstein equations.

Quantum gravity being an unfinished symphony, we cannot entirely conclude how great an impact knot theory will have on it in the end. One can only note that beautiful mathematical results seem to tie in naturally with the partial constructions that have been carried out thus far.

See also: BF Theories; Braided and Modular Tensor Categories; Finite-Type Invariants; Finite-type invariants of 3-Manifolds; The Jones Polynomial; Knot Theory and Physics; Loop Quantum Gravity; Mathematical Knot Theory; Quantum Dynamics in Loop Quantum Gravity; Quantum Geometry and its Applications; Yang–Baxter Equations.

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Knot Theory and Physics

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Introduction

This article is an introduction to some of the relationships between knot theory and theoretical physics. Knots themselves are macroscopic physical phenomena in three-dimensional space, occurring in rope, vines, telephone cords, polymer chains, DNA, certain species of eel, and many other places in the natural and manmade world. The study of topological invariants of knots leads to relationships with statistical mechanics and quantum physics. This is a remarkable and deep situation where the study of a certain (topological) aspects of the macroscopic world is entwined with theories developed for the subtleties of the microscopic world. The present article is an introduction to the mathematical side of these connections, with some hints and references to the related physics.

We begin with a short introduction to knots, links, braids, and the bracket polynomial invariant of knots and links. The article then discusses Vassiliev invariants of knots and links, and how these invariants are naturally related to Lie algebras and to Witten's gauge-theoretic approach. This part

of the article is an introduction to how Vassiliev invariants in knot theory arise naturally in the context of Witten's functional integral.

The article is divided into several sections beyond the introduction. Section two is a quick introduction to the topology of knots and links. The third one discusses Vassiliev invariants and invariants of rigid vertex graphs. The fourth section introduces the basic formalism and shows how Witten's functional integral is related directly to Vassiliev invariants. The fifth section discusses the loop transform and loop quantum gravity in this context. The final section is an introduction to topological quantum field theory, and to the use of these techniques in producing unitary representations of the braid group, a topic of intense interest in quantum information theory.

Knots, Braids, and Bracket Polynomial

The purpose of this section is to give a quick introduction to the diagrammatic theory of knots, links, and braids. A knot is an embedding of a circle in three-dimensional space, taken up to ambient isotopy. That is, two knots are regarded as equivalent if one embedding can be obtained from the other through a continuous family of embeddings of circles in 3-space. A link is an embedding of a disjoint collection of circles, taken up to ambient isotopy. **Figure 1** illustrates a diagram for a knot. The diagram is regarded both as a schematic picture of the knot, and as a plane graph with extra structure at the nodes (indicating how the curve of the knot passes over or under itself by standard pictorial conventions).

Ambient isotopy is mathematically the same as the equivalence relation generated on diagrams by the Reidemeister moves. These moves are illustrated in **Figure 2**. Each move is performed on a local part of the diagram that is topologically identical to the part of the diagram illustrated in this figure (these figures are representative examples of the types of Reidemeister moves) without changing the rest of the diagram. The Reidemeister moves are useful in

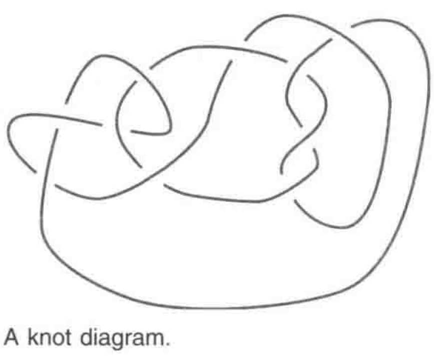


Figure 1 A knot diagram.

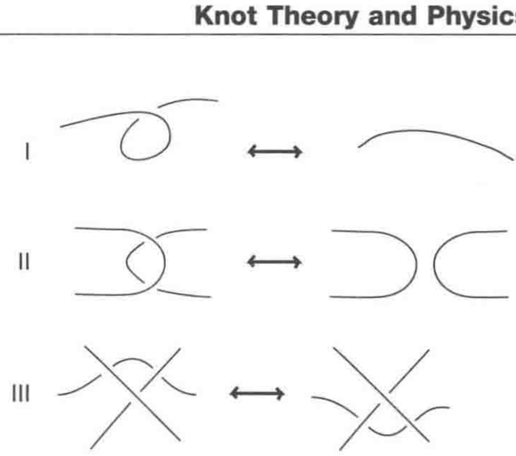


Figure 2 The Reidemeister moves.

doing combinatorial topology with knots and links, notably in working out the behavior of knot invariants. A knot invariant is a function defined from knots and links to some other mathematical object (such as groups or polynomials or numbers) such that equivalent diagrams are mapped to equivalent objects (isomorphic groups, identical polynomials, identical numbers).

Another significant structure related to knots and links is the Artin braid group. A braid is an embedding of a collection of strands that have their ends in two rows of points that are set one above the other with respect to a choice of vertical. The strands are not individually knotted and they are disjoint from one another. See **Figures 3–5** for illustrations of braids and moves on braids. Braids can be multiplied by attaching the bottom row of one braid to the top row of the other braid. Taken up to ambient isotopy, fixing the endpoints, the braids form a group under this notion of multiplication. In **Figure 3** we illustrate the form of the basic generators of the braid group, and the form of the relations among these generators. **Figure 4** illustrates how to close a braid by attaching the top strands to the bottom strands by a collection of parallel arcs. A key theorem of Alexander states that every knot or link can be represented as a closed braid. Thus, the theory of braids is critical to the

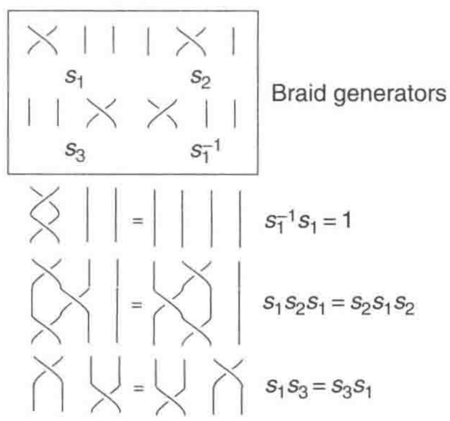


Figure 3 Braid generators.

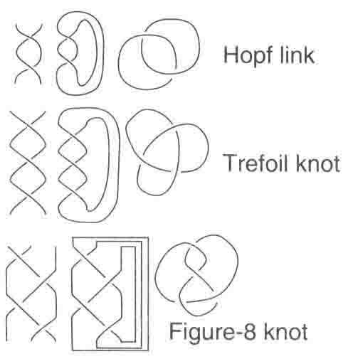


Figure 4 Closing braids to form knots and links.

theory of knots and links. **Figure 5** illustrates the famous Borrowmean rings (a link of three unknotted loops such that any two of the loops are unlinked) as the closure of a braid.

We now discuss a significant example of an invariant of knots and links, the bracket polynomial. The bracket polynomial can be normalized to produce an invariant of all the Reidemeister moves. This normalized invariant is known as the Jones (1985) polynomial. The Jones polynomial was originally discovered by a different method than the one given here.

The bracket polynomial, $\langle K\rangle = \langle K\rangle(A)$, assigns to each unoriented link diagram K a Laurent polynomial in the variable A, such that

1. If K and K' are regularly isotopic diagrams, then $\langle K\rangle = \langle K'\rangle$.
2. If K II O denotes the disjoint union of K with an extra unknotted and unlinked component O (also called "loop" or "simple closed curve" or "Jordan curve"), then

$$\langle K\ \mathrm{II}\ O\rangle = \delta\langle K\rangle$$

where

$$\delta = -A^2 - A^{-2}$$

3. $\langle K\rangle$ satisfies the following formulas:

$$\langle \chi\rangle = A\langle \asymp\rangle + A^{-1}\langle)(\rangle$$
$$\langle \overline{\chi}\rangle = A^{-1}\langle \asymp\rangle + A\langle)(\rangle$$

where the small diagrams represent parts of larger diagrams that are identical except at the site indicated in the bracket. We take the convention that the letter chi, χ, denotes a crossing where the curved line is crossing over the straight segment. The barred letter denotes the switch of this crossing, where the curved line is undercrossing the straight segment.

In computing the bracket, one finds the following behavior under Reidemeister move I:

$$\langle \gamma\rangle = -A^3\langle \smile\rangle$$

and

$$\langle \overline{\gamma}\rangle = -A^{-3}\langle \smile\rangle$$

where γ denotes a curl of positive type as indicated in **Figure 6**, and $\overline{\gamma}$ indicates a curl of negative type, as also seen in this figure. The type of a curl is the sign of the crossing when we orient it locally. Our convention of signs is also given in **Figure 6**. Note that the type of a curl does not depend on the orientation we choose. The small arcs on the right-hand side of these formulas indicate the removal of the curl from the corresponding diagram.

The bracket is invariant under regular isotopy and can be normalized to an invariant of ambient isotopy by the definition

$$f_K(A) = (-A^3)^{-w(K)}\langle K\rangle(A)$$

where we chose an orientation for K, and where $w(K)$ is the sum of the crossing signs of the oriented link K. $w(K)$ is called the writhe of K. The convention for crossing signs is shown in **Figure 6**.

The State Summation

In order to obtain a closed formula for the bracket, we now describe it as a state summation. Let K be any unoriented link diagram. Define a state, S, of K to be a choice of smoothing for each crossing of K. There are two choices for smoothing a given crossing, and thus there are 2^N states of a diagram with N crossings. In a state we label each smoothing with A or A^{-1} as in the expansion formula for the bracket. The label is called a vertex weight of the

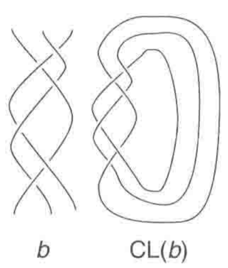


Figure 5 Borromean rings as a braid closure.

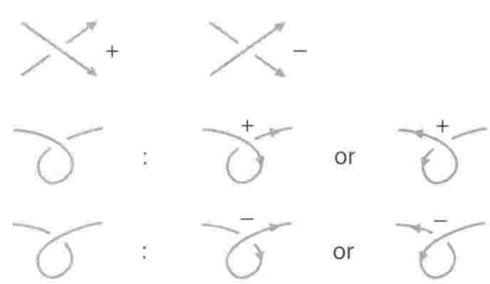


Figure 6 Crossing signs and curls.

state. There are two evaluations related to a state. The first one is the product of the vertex weights, denoted $\langle K|S\rangle$. The second evaluation is the number of loops in the state S, denoted $\|S\|$.

Define the state summation, $\langle K\rangle$, by the formula

$$\langle K\rangle = \sum_S \langle K|S\rangle \delta^{\|S\|-1}$$

It follows from this definition that $\langle K\rangle$ satisfies the equations

$$\langle \chi\rangle = A\langle \asymp\rangle + A^{-1}\langle)(\rangle$$
$$\langle K \amalg O\rangle = \delta\langle K\rangle$$
$$\langle O\rangle = 1$$

The first equation expresses the fact that the entire set of states of a given diagram is the union, with respect to a given crossing, of those states with an A-type smoothing and those with an A^{-1}-type smoothing at that crossing. The second and the third equation are clear from the formula defining the state summation. Hence, this state summation produces the bracket polynomial as we have described it at the beginning of the section.

Remark By a change of variables one obtains the original Jones polynomial, $V_K(t)$, for oriented knots and links from the normalized bracket:

$$V_K(t) = f_K(t^{-1/4})$$

Remark The bracket polynomial provides a connection between knot theory and physics, in that the state summation expression for it exhibits it as a generalized partition function defined on the knot diagram. Partition functions are ubiquitous in statistical mechanics, where they express the summation over all states of the physical system of probability weighting functions for the individual states. Such physical partition functions contain large amounts of information about the corresponding physical system. Some of this information is directly present in the properties of the function, such as the location of critical points and phase transition. Some of the information can be obtained by differentiating the partition function, or performing other mathematical operations on it.

In fact, by defining a generalization of the bracket polynomial, defined on knot diagrams but not invariant under the Reidemeister moves, we can capture significant partition functions that are physically meaningful. There is no room in this survey to detail how this generalization can be used to express the Potts model for planar graphical configurations, and how it expresses the relationship between the Potts model and the Temperley–Lieb algebra in diagrammatic form. There is much more in this connection with statistical mechanics in that the local weights in a partition function are often expressed in terms of solutions to a matrix equation called the Yang–Baxter equation, that turns out to fit perfectly invariance under the third Reidemeister move. As a result, there are many ways to define partition functions of knot diagrams that give rise to invariants of knots and links. The subject is intertwined with the algebraic structure of Hopf algebras and quantum groups, useful for producing systematic solutions to the Yang–Baxter equation. In fact, Hopf algebras are deeply connected with the problem of constructing invariants of three-dimensional manifolds in relation to invariants of knots. We have chosen, in this survey article, not to discuss the details of these approaches, but rather to proceed to Vassiliev invariants and the relationships with Witten's functional integral. The reader is referred to Kauffman (1987, 1994, 2002), Jones (1985), and Reshetikhin and Turaev (1991) for more information about relationships of knot theory with statistical mechanics, Hopf algebras, and quantum groups. For topology, the key point is that Lie algebras can be used to construct invariants of knots and links. This is shown nowhere more clearly than in the theory of Vassiliev invariants that we take up in the next section.

Vassiliev Invariants and Invariants of Rigid Vertex Graphs

In this section we study the combinatorial topology of Vassiliev invariants. As we shall see, by the end of this section, Vassiliev invariants are directly connected with Lie algebras, and representations of Lie algebras can be used to construct them. This aspect of link invariants is one of the most fundamental for connections with physics. Just as symmetry considerations in physics lead to a fundamental relationship with Lie algebras, topological invariance leads to a fundamental relationship of the theory of knots and links with Lie algebras.

If $V(K)$ is a (Laurent polynomial valued or, more generally, commutative ring valued) invariant of knots, then it can be naturally extended to an invariant of rigid vertex graphs by defining the invariant of graphs in terms of the knot invariant via an "unfolding of the vertex." That is, we can regard the vertex as a "black box" and replace it by any tangle of our choice. Rigid vertex motions of the graph preserve the contents of the black box, and hence implicate ambient isotopies of the link obtained by replacing the black box by its contents.

Invariants of knots and links that are evaluated on these replacements are then automatically rigid vertex invariants of the corresponding graphs. If we set up a collection of multiple replacements at the vertices with standard conventions for the insertions of the tangles, then a summation over all possible replacements can lead to a graph invariant with new coefficients corresponding to the different replacements. In this way, each invariant of knots and links implicates a large collection of graph invariants.

The simplest tangle replacements for a 4-valent vertex are the two crossings, positive and negative, and the oriented smoothing. Let $V(K)$ be any invariant of knots and links. Extend V to the category of rigid vertex embeddings of 4-valent graphs by the formula

$$V(K_*) = aV(K_+) + bV(K_-) + cV(K_0)$$

where K_+ denotes a knot diagram K with a specific choice of positive crossing, K_- denotes a diagram identical to the first with the positive crossing replaced by a negative crossing and K_* denotes a diagram identical to the first with the positive crossing replaced by a graphical node.

There is a rich class of graph invariants that can be studied in this manner. The Vassiliev invariants (Bar-Natan 1995) constitute the important special case of these graph invariants where $a = +1, b = -1$ and $c = 0$. Thus, $V(G)$ is a Vassiliev invariant if

$$V(K_*) = V(K_+) - V(K_-)$$

Call this formula the exchange identity for the Vassiliev invariant V. See **Figure 7**.

V is said to be of finite type k if $V(G) = 0$ whenever $|G| > k$, where $|G|$ denotes the number of (4-valent) nodes in the graph G. The notion of finite type is of extraordinary significance in studying these invariants. One reason for this is the following basic lemma.

Lemma *If a graph G has exactly k nodes, then the value of a Vassiliev invariant v_k of type k on G, $v_k(G)$, is independent of the embedding of G.*

Proof Omitted. □

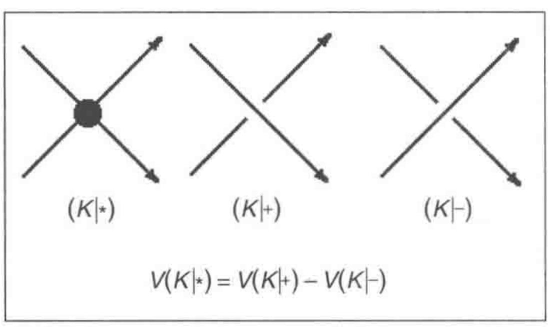


Figure 7 Exchange identity for Vassiliev invariants.

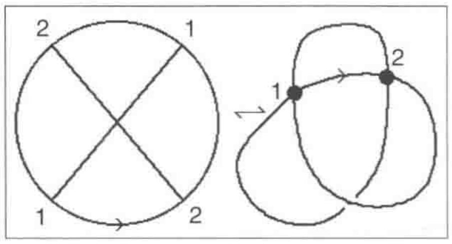


Figure 8 Chord diagrams.

The upshot of this lemma is that Vassiliev invariants of type k are intimately involved with certain abstract evaluations of graphs with k nodes. In fact, there are restrictions (the four-term relations) on these evaluations demanded by the topology and it follows from results of Kontsevich (see Bar-Natan (1995) that such abstract evaluations actually determine the invariants. The knot invariants derived from classical Lie algebras are all built from Vassiliev invariants of finite type. All of this is directly related to Witten's functional integral (Witten 1989).

In the next few figures we illustrate some of these main points. In **Figure 8** we show how one associates a so-called chord diagram to represent the abstract graph associated with an embedded graph. The chord diagram is a circle with arcs connecting those points on the circle that are welded to form the corresponding graph. In **Figure 9** we illustrate how the four-term relation is a consequence of topological invariance.

In **Figure 10** we show how the four-term relation is a consequence of the abstract pattern of the commutator

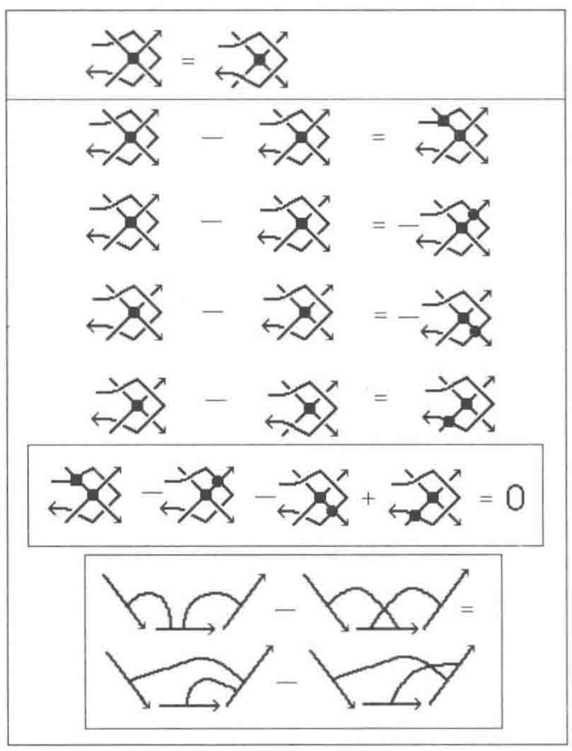


Figure 9 The four-term relation from topology.

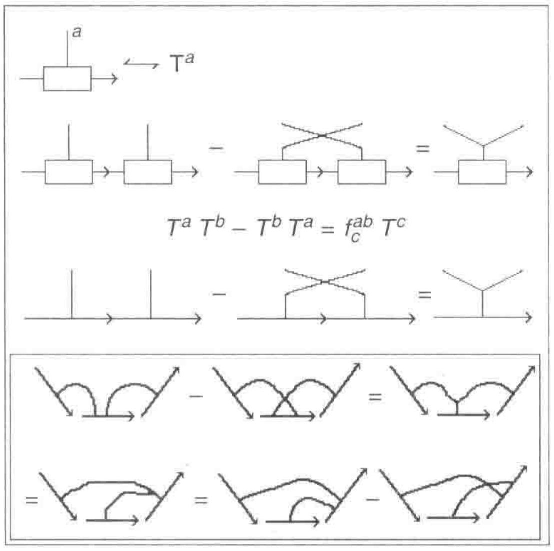


Figure 10 The four-term relation from categorical Lie algebra.

identity for a matrix Lie algebra. That is, we show how a diagrammatic version of the formula

$$T^aT^b - T^bT^a = f_c^{ab}T^c$$

fits directly with the four-term relation. The formula we have quoted here states that the commutator of the matrices T^a and T^b is equal to a sum of the matrices T^c with coefficients (the structure coefficients of the Lie algebra) f_c^{ab}. Such a relation is the most concrete way to define a matrix Lie algebra. There are other levels of abstraction that can be employed here. The same diagrammatic can be interpreted directly in terms of the Jacobi identity that defines a Lie algebra. We shall content ourselves with this matrix point of view here, and add that it is assumed here that the structure coefficients are invariant under cyclic permutation, an assumption that is not needed in the general case. The four-term relation is directly related to a categorical generalization of Lie algebras.

Figure 11 illustrates how the weights are assigned to the chord diagrams in the Lie algebra case – by inserting Lie algebra matrices into the circle and taking a trace of a sum of matrix products. The relationship between Vassiliev invariants and Lie algebras has been known since Bar-Natan's thesis (see also Kauffman (1995). In Bar-Natan (1995) the reader will find a good account of Kontsevich's theorem, showing how Lie algebra weight systems, and in fact any weight system satisfying the four-term relation, can be used to construct knot invariants. Conceptually, the ideas behind the Kontsevich theorem are directly related to Witten's approach to knot invariants via quantum field theory. We give an exposition of this approach in the next section of this article.

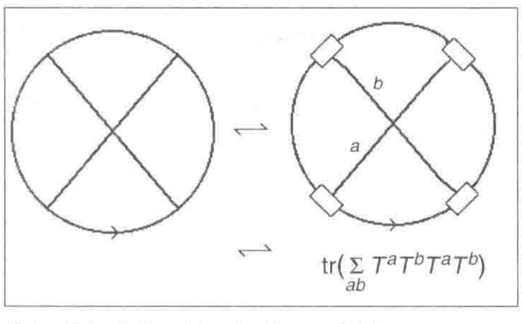


Figure 11 Calculating Lie algebra weights.

Example Let $P_K(t) = f_K(e^t)$ $(A = e^t)$ where $f_K(A)$ is the normalized bracket polynomial invariant discussed in the last section. Then $P_K(t)$ is expressed as a power series in t with coefficients $v_n(K)$, $n = 0, 1, 2, \ldots$, that are invariants of the knot or link K. It is not hard to show that these coefficient invariants (extended to graphs so that the Vassiliev exchange identity is satisfied) are Vassiliev invariants of finite type. In fact, most of the so-called polynomial invariants of knots and links (relatives of the bracket and Jones polynomials) give rise to Vassiliev invariants in just this way. Thus, Vassiliev invariants of finite type are ubiquitous in this area of knot theory. One can think of Vassiliev invariants as building blocks for the other invariants, or that these invariants are sources of Vassiliev invariants.

Vassiliev Invariants and Witten's Functional Integral

Edward Witten (1989) proposed a formulation of a class of 3-manifold invariants as generalized Feynman integrals taking the form $Z(M)$, where

$$Z(M) = \int DAe^{(ik/4\pi)S(M,A)}$$

Here M denotes a 3-manifold without boundary and A is a gauge field (also called a gauge potential or gauge connection) defined on M. The gauge field is a 1-form on a trivial G-bundle over M with values in a representation of the Lie algebra of G. The group G corresponding to this Lie algebra is said to be the gauge group. In this integral, the action $S(M, A)$ is taken to be the integral over M of the trace of the Chern–Simons 3-form $A \wedge dA + (2/3)A \wedge A \wedge A$. (The product is the wedge product of differential forms.) $Z(M)$ integrates over all gauge fields modulo gauge equivalence.

The formalism and internal logic of Witten's integral supports the existence of a large class of topological invariants of 3-manifolds and associated invariants of knots and links in these manifolds.

The invariants associated with this integral have been given rigorous combinatorial descriptions but questions and conjectures arising from the integral formulation are still outstanding. Specific conjectures about this integral take the form of just how it implicates invariants of links and 3-manifolds, and how these invariants behave in certain limits of the coupling constant k in the integral. Many conjectures of this sort can be verified through the combinatorial models. On the other hand, the really outstanding conjecture about the integral is that it exists! At the present time there is no measure theory or generalization of measure theory that supports it in full generality. Here is a formal structure of great beauty. It is also a structure whose consequences can be verified by a remarkable variety of alternative means.

The formalism of the Witten integral implicates invariants of knots and links corresponding to each classical Lie algebra. In order to see this, we need to introduce the Wilson loop. The Wilson loop is an exponentiated version of integrating the gauge field along a loop K in three space that we take to be an embedding (knot) or a curve with transversal self-intersections. For this discussion, the Wilson loop will be denoted by the notation

$$W_K(A)$$

to denote the dependence on the loop K and the field A. It is usually indicated by the symbolism $\mathrm{tr}(Pe^{\oint_K A})$. Thus,

$$W_K(A) = \mathrm{tr}\left(Pe^{\oint_K A}\right)$$

Here the P denotes path ordered integration – we are integrating and exponentiating matrix valued functions, and so must keep track of the order of the operations. The symbol tr denotes the trace of the resulting matrix. This Wilson loop integration exists by normal means and does not require functional integration.

With the help of the Wilson loop functional on knots and links, Witten writes down a functional integral for link invariants in a 3-manifold M:

$$\begin{aligned} Z(M,K) &= \int DAe^{(ik/4\pi)S(M,A)}\mathrm{tr}\left(Pe^{\oint_K A}\right) \\ &= \int DAe^{(ik/4\pi)S}W_K(A) \end{aligned}$$

Here $S(M,A)$ is the Chern–Simons Lagrangian, as in the previous discussion. We abbreviate $S(M,A)$ as S and write $W_K(A)$ for the Wilson loop. Unless otherwise mentioned, the manifold M will be the three-dimensional sphere S^3.

An analysis of the formalism of this functional integral reveals quite a bit about its role in knot theory. One can determine how the Witten integral behaves under a small deformation of the loop K.

Theorem

(i) *Let* $Z(K)=Z(S^3,K)$ *and let* $\delta Z(K)$ *denote the change of* $Z(K)$ *under an infinitesimal change in the loop* K. *Then*

$$\delta Z(K) = (4\pi i/k)\int dAe^{(ik/4\pi)S}[\mathrm{Vol}]T_aT_aW_K(A)$$

where $\mathrm{Vol}=\epsilon_{rst}dx^r dx^s dx^t$.

The sum is taken over repeated indices, and the insertion is taken of the matrices T_aT_a *at the chosen point* x *on the loop* K *that is regarded as the center of the deformation. The volume element* $\mathrm{Vol}=\epsilon_{rst}dx_r dx_s dx_t$ *is taken with regard to the infinitesimal directions of the loop deformation from this point on the original loop.*

(ii) *The same formula applies, with a different interpretation, to the case where* x *is a double point of transversal self-intersection of a loop* K, *and the deformation consists in shifting one of the crossing segments perpendicularly to the plane of intersection so that the self-intersection point disappears. In this case, one* T_a *is inserted into each of the transversal crossing segments so that* $T_aT_aW_K(A)$ *denotes a Wilson loop with a self-intersection at* x *and insertions of* T_a *at* $x+\epsilon_1$ *and* $x+\epsilon_2$, *where* ϵ_1 *and* ϵ_2 *denote small displacements along the two arcs of* K *that intersect at* x. *In this case, the volume form is nonzero, with two directions coming from the plane of movement of one arc, and the perpendicular direction is the direction of the other arc.*

Remark One shows that the result of a topological variation has an analytic expression that is zero if the topological variation does not create a local volume. Thus, we have shown that the integral of $e^{(ik/4\pi)S(A)}W_K(A)$ is topologically invariant as long as the curve K is moved by the local equivalent of regular isotopy.

In the case of switching a crossing, the key point is to write the crossing switch as a composition of first moving a segment to obtain a transversal intersection of the diagram with itself, and then to continue the motion to complete the switch. Up to the choice of our conventions for constants, the switching formula is, as shown below (see **Figure 12**).

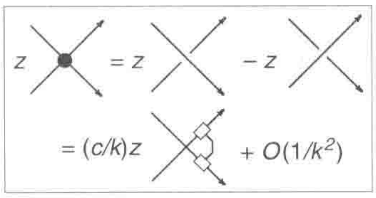


Figure 12 The difference formula.

$$\begin{aligned} &Z(K_+) - Z(K_-) \\ &= (4\pi i/k) \int DA e^{(ik/4\pi)S} T_a T_a \langle K_{**}|A\rangle \\ &= (4\pi i/k) Z(T^a T^a K_{**}) \end{aligned}$$

where K_{**} denotes the result of replacing the crossing by a self-touching crossing. We distinguish this from adding a graphical node at this crossing by using the double-star notation.

A key point is to notice that the Lie algebra insertion for this difference is exactly what is done (in chord diagrams) to make the weight systems for Vassiliev invariants (without the framing compensation). Thus, the formalism of the Witten functional integral takes one directly to these weight systems in the case of the classical Lie algebras. In this way, the functional integral is central to the structure of the Vassiliev invariants.

The Loop Transform and Quantum Gravity

Suppose that $\psi(A)$ is a (complex-valued) function defined on gauge fields. Then we define formally the loop transform $\widehat{\psi}(K)$, a function on embedded loops in three-dimensional space, by the formula

$$\widehat{\psi}(K) = \int DA \psi(A) W_K(A)$$

If Δ is a differential operator defined on $\psi(A)$, then we can use this integral transform to shift the effect of Δ to an operator on loops via integration by parts:

$$\begin{aligned} \widehat{\Delta\psi}(K) &= \int DA \Delta\psi(A) W_K(A) \\ &= -\int DA \psi(A) \Delta W_K(A) \end{aligned}$$

When Δ is applied to the Wilson loop, the result can be an understandable geometric or topological operation. One can illustrate this situation with operators G and H:

$$\begin{aligned} G &= -F^a_{ij} dx^i \delta/\delta A^a_j(x) \\ H &= -\epsilon_{ars} F^a_{ij} \delta/\delta A^s_i \delta/\delta A^r_j \end{aligned}$$

with summation over the repeated indices. Each of these operators has the property that its action on the Wilson loop has a geometric or topological interpretation. One has

$$\widehat{G\psi}(K) = \delta\widehat{\psi}(K)$$

where this variation refers to the effect of varying K. As we saw in the previous section, this means that if $\widehat{\psi}(K)$ is a topological invariant of knots and links, then $\widehat{G\psi}(K) = 0$ for all embedded loops K. This condition is a transform analog of the equation $G\psi(A) = 0$. This equation is the differential analog of an invariant of knots and links. It may happen that $\delta\widehat{\psi}(K)$ is not strictly zero, as in the case of our framed knot invariants. For example, with

$$\psi(A) = \exp\left((ik/4\pi) \int tr(A \wedge dA + (2/3) A \wedge A \wedge A)\right)$$

we conclude that $\widehat{G\psi}(K)$ is zero for flat deformations (in the sense of the previous section) of the loop K, but can be nonzero in the presence of a twist or curl. In this sense, the loop transform provides a subtle variation on the strict condition $G\psi(A) = 0$.

In Ashtekar *et al.* (1992) and other publications by Ashtekar, Rovelli, Smolin, and their colleagues, the loop transform is used to study a reformulation and quantization of Einstein gravity. The differential-geometric gravity theory of Einstein is reformulated in terms of a background gauge connection and in the quantization, the Hilbert space consists in functions $\psi(A)$ that are required to satisfy the constraints $G\psi = 0$ and $H\psi = 0$. Thus, we see that $\widehat{G}(K)$ can be partially zero in the sense of producing a framed knot invariant, and that $\widehat{H}(K)$ is zero for non-self-intersecting loops. This means that the loop transforms of G and H can be used to investigate a subtle variation of the original scheme for the quantization of gravity. This program is being actively pursued by a number of researchers. The Vassiliev invariants arising from a topologically invariant loop transform are of significance to this theory.

Braiding, Topological Quantum Field Theory, and Quantum Computing

The purpose of this section is to discuss in a very general way how braiding is related to topological quantum field theory and to the enterprise (Freedman *et al.* 2002) of using this sort of theory as a model for anyonic quantum computation. The ideas in the subject of topological quantum field theory are well expressed by Michael Atiyah (1990)

and Edward Witten (1989). The simplest case of this idea is C N Yang's original interpretation of the Yang–Baxter equation. Yang articulated a quantum field theory in one dimension of space and one dimension of time, in which the R-matrix giving the scattering amplitudes for an interaction of two particles whose (let us say) spins corresponded to the matrix indices so that R_{ab}^{cd} is the amplitude for particles of spin a and spin b to interact and produce particles of spin c and d. Since these interactions are between particles in a line, one takes the convention that the particle with spin a is to the left of the particle with spin b, and the particle with spin c is to the left of the particle with spin d. If one follows the concatenation of such interactions, then there is an underlying permutation that is obtained by following strands from the bottom to the top of the diagram (thinking of time as moving up the page). Yang designed the Yang–Baxter equation for R so that the amplitudes for a composite process depend only on the underlying permutation corresponding to the process and not on the individual sequences of interactions.

In taking over the Yang–Baxter equation for topological purposes, we can use the same interpretation, but think of the diagrams with their under- and over-crossings as modeling events in a spacetime with two dimensions of space and one dimension of time. The extra spatial dimension is taken in displacing the woven strands perpendicular to the page, and allows the use of braiding operators R and R^{-1} as scattering matrices. Taking this picture to heart, one can add other particle properties to the idealized theory. In particular, one can add fusion and creation vertices where, in fusion, two particles interact to become a single particle and, in creation, one particle changes (decays) into two particles. Matrix elements corresponding to trivalent vertices can represent these interactions (see **Figure 13**).

Once one introduces trivalent vertices for fusion and creation, there is the question how these interactions will behave in respect to the braiding operators. There will be a matrix expression for the compositions of braiding and fusion or creation as indicated in **Figure 14**. Here we will restrict ourselves to showing the diagrammatics with the intent of giving the reader a flavor of these

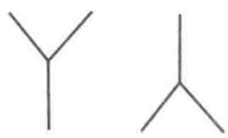


Figure 13 Creation and fusion.

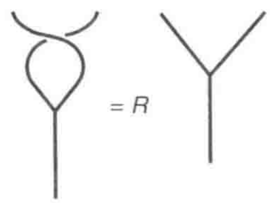


Figure 14 Braiding.

structures. It is natural to assume that braiding intertwines with creation as shown in **Figure 15** (similarly with fusion). This intertwining identity is clearly the sort of thing that a topologist will love, since it indicates that the diagrams can be interpreted as embeddings of graphs in three-dimensional space. **Figure 16** illustrates the Yang–Baxter equation. The intertwining identity is an assumption like the Yang–Baxter equation itself, which simplifies the mathematical structure of the model.

It is to be expected that there will be an operator that expresses the recoupling of vertex interactions as shown in **Figure 17** and labeled by Q. The actual formalism of such an operator will parallel the mathematics of recoupling for angular momentum (see, e.g., Kauffman (1994)). If one just considers the abstract structure of recoupling then one sees that for trees with four branches (each with a single root) there is a cycle of length 5, as shown in

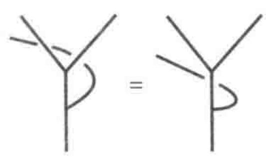


Figure 15 Intertwining.

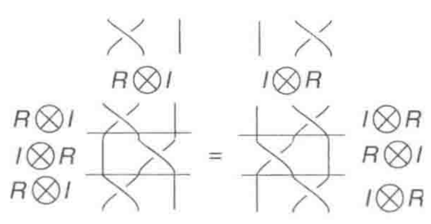


Figure 16 Yang–Baxter equation.

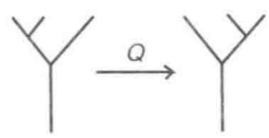


Figure 17 Recoupling.

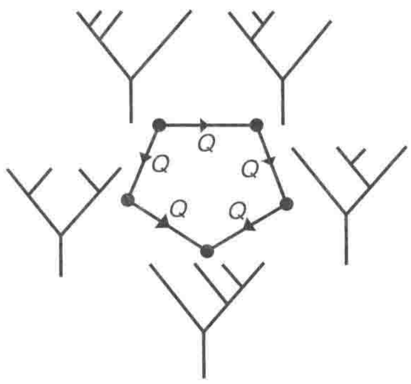


Figure 18 Pentagon identity.

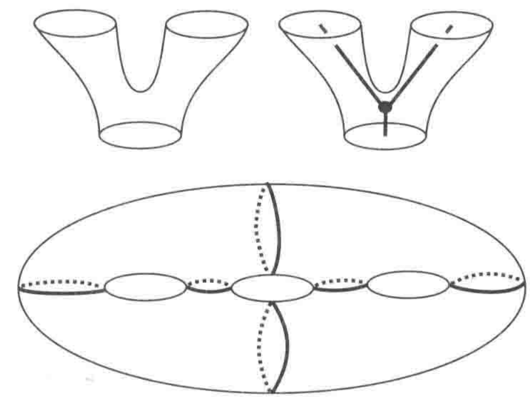


Figure 20 Decomposition of a surface into trinions.

Figure 17. One can start with any pattern of three vertex interactions and go through a sequence of five recouplings that bring one back to the same tree from which one started. It is a natural simplifying axiom to assume that this composition is the identity mapping. This axiom is called the pentagon identity (**Figure 18**).

Finally, there is a hexagonal cycle of interactions between braiding, recoupling and the intertwining identity as shown in **Figure 19**. One says that the interactions satisfy the hexagon identity if this composition is the identity.

A three-dimensional topological quantum field theory is an algebra of interactions that satisfies the Yang–Baxter equation, the intertwining identity, the pentagon identity and the hexagon identity. There is no room in this summary to detail the way that these properties fit into the topology of knots and three-dimensional manifolds, but a sketch is in order. For the case of topological quantum field theory related to the group SU(2) there is a construction based entirely on the combinatorial topology of the bracket polynomial (see the section

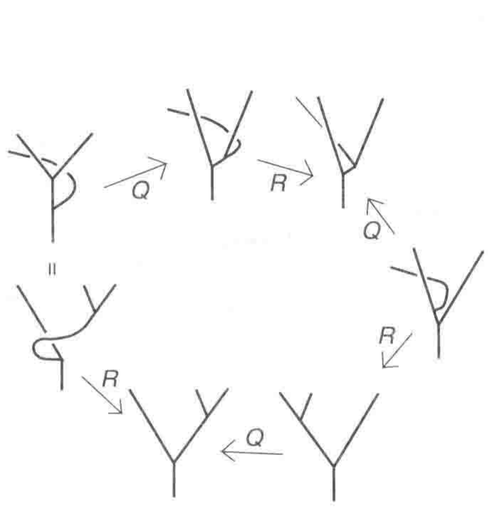


Figure 19 Hexagon identity.

"Knots, braids, and bracket polynomial"). For more information on this approach, the reader is referred to Kauffman (1994, 2002).

It turns out that the algebraic properties of a topological quantum field theory give it enough power to rigourously model three manifold invariants described by the Witten integral. This is done by regarding the 3-manifold as a union of two handlebodies with boundary an orientable surface S_g of genus g. The surface is divided up into trinions as illustrated in **Figure 20**. A trinion is a surface with boundary that is topologically equivalent to a sphere with three punctures. In **Figure 20** we illustrate two trinions, the second shown as a neighborhood of a trivalent vertex, and a surface of genus 3 that is decomposed into three trinions. It turns out that there is a way to associate a vector space $V(S_g)$ to a surface with a trinion decomposition, defined in terms of the associated topological quantum field theory, such that the isomorphism class of the vector space $V(S_g)$ does not depend upon the choice of decomposition. This independence is guaranteed by the braiding, hexagon, and pentagon identities in such a way that one can associate a well-defined vector $|M_\epsilon\rangle$ in $V(S_g)$ whenever M is a 3-manifold whose boundary is S_g. Furthermore, if a closed 3-manifold M^3 is decomposed along a surface S_g into the union of M_- and M_+, where these parts are otherwise disjoint 3-manifolds with boundary S_g, then the inner product $I(M) = \langle M_- | M_+ \rangle$ is, up to normalization, an invariant of the 3-manifold M_3. With the definition of topological quantum field theory given above, knots and links can be incorporated as well, so that one obtains a source of invariants $I(M^3, K)$ of knots and links in orientable 3-manifolds.

The invariant $I(M^3, K)$ can be formally compared with the Witten integral

$$Z(M^3, K) = \int DA e^{(ik/4\pi)S(M,A)} W_K(A)$$

It can be shown that up to limits of the heuristics, $Z(M, K)$ and $I(M^3, K)$ are essentially equivalent for appropriate choice of gauge groups.

This point of view leads to more abstract formulations of topological quantum field theories as ways to associate vector spaces and linear transformations to manifolds and cobordisms of manifolds. (A cobordism of surfaces is a 3-manifold whose boundary consists of these surfaces.)

As the reader can see, a three-dimensional TQFT is, at base, a highly simplified theory of point-particle interactions in $(2+1)$-dimensional spacetime. It can be used to articulate invariants of knots and links and invariants of 3-manifolds. The reader interested in the SU(2) case of this structure and its implications for invariants of knots and 3-manifolds can consult Kauffman (1994, 2002) and Crane (1991). One expects that physical situations involving $2+1$ spacetime will be approximated by such an idealized theory. It is thought, for example, that aspects of the quantum Hall effect will be related to topological quantum field theory (Wilczek 1990). One can imagine a physics where the geometrical space is two dimensional and the braiding of particles corresponds to their interactions through circulating around one another in the plane. Anyons are particles that do not just change their wave functions by a sign under interchange, but rather by a complex phase or even a linear combination of states. It is hoped that TQFT models will describe applicable physics. One can think about the possible applications of anyons to quantum computing. The TQFTs then provide a class of anyonic models where the braiding is essential to the physics and to the quantum computation.

The key point in the application and relationship of TQFT and quantum information theory is, in our opinion, contained in the structure illustrated in **Figure 21**. There we show a more complex braiding operator, based on the composition of recoupling with the elementary braiding at a vertex. (This structure is implicit in the hexagon identity of **Figure 19**.) The new braiding operator is a source of unitary representations of braid group in situations (which exist mathematically) where the recoupling transformations are themselves unitary. This kind of pattern is utilized in the work of Freedman *et al.* (2002) and in the case of classical angular momentum formalism has been dubbed a "spin-network quantum simulator" by Rasetti and collaborators (see, e.g., Marzuoli and Rasetti (2002). Kauffman and Lomonaco (2006) show how certain natural deformations (Kauffman 1994) of Penrose (1969) spin networks can be used to produce such the Freedman–Kitaev model for anyonic topological quantum computation. It is legitimate to speculate that networks of this kind are present in physical reality.

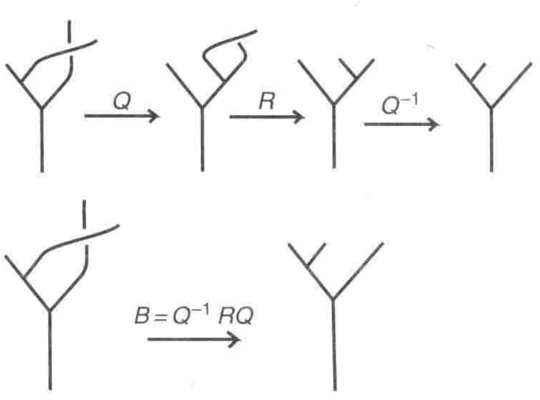


Figure 21 A more complex braiding operator.

Quantum computing can be regarded as a study of the structure of the preparation, evolution, and measurement of quantum systems. In the quantum computation model, an evolution is a composition of unitary transformations (usually finite-dimensional over the complex numbers). The unitary transformations are applied to an initial state vector that has been prepared prior to this process. Measurements are projections to elements of an orthonormal basis of the space upon which the evolution is applied. The result of measuring a state $|\psi\rangle$, written in the given basis, is probabilistic. The probability of obtaining a given basis element from the measurement is equal to the absolute square of the coefficient of that basis element in the state being measured.

It is remarkable that the above lines constitute an essential summary of quantum theory. All applications of quantum theory involve filling in details of unitary evolutions and specifics of preparations and measurements. Such unitary evolutions can be seen as approximated arbitrarily closely by representations of the Artin braid group. The key to the anyonic models of quantum computation via topological quantum field theory, or via deformed spin networks, is that all unitary evolutions can be approximated by a single coherent method for producing representations of the braid group. This beautiful mathematical fact points to a deep role for topology in the structure of quantum physics.

The future of knots, links, and braids in relation to physics will be very exciting. There is no question that unitary representations of the braid group and quantum invariants of knots and links play a fundamental role in the mathematical structure of quantum mechanics, and we hope that time will show us the full meaning of this relationship.

Acknowledgments

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See also: Chern–Simons Models: Rigorous Results; Functional Integration in Quantum Physics; Knot Homologies; Knot Invariants and Quantum Gravity; Large-*N* and Topological Strings; Loop Quantum Gravity; Mathematical Knot Theory; Schwarz-Type Topological Quantum Field Theory; The Jones Polynomial; Topological Knot Theory and Macroscopic Physics; Topological Quantum Field Theory: Overview; Two-Dimensional Conformal Field Theory and Vertex Operator Algebras; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory; Yang–Baxter Equations.

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Kontsevich Integral

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Introduction

The Kontsevich integral was invented by Kontsevich (1993) as a tool to prove the fundamental theorem of the theory of finite-type (Vassiliev) invariants (see Bar-Natan (1995a)). It provides an invariant exactly as strong as the totality of all Vassiliev knot invariants.

The Kontsevich integral is defined for oriented tangles (either framed or unframed) in $\mathbb{R}^3$; therefore, it is also defined in the particular cases of knots, links, and braids (see **Figure 1**).

As a starter, we give two examples where simple versions of the Kontsevich integral have a straightforward geometrical meaning. In these examples, as well as in the general construction of the Kontsevich integral, we represent 3-space $\mathbb{R}^3$ as the product of a real line $\mathbb{R}$ with coordinate t and a complex plane $\mathbb{C}$ with complex coordinate z.

Example 1 The number of twists in a braid with two strings $z_1(t)$ and $z_2(t)$ placed in the slice $0 \leq t \leq 1$ (see **Figure 2**) is equal to

$$\frac{1}{2\pi i}\int_0^1 \frac{dz_1 - dz_2}{z_1 - z_2}$$

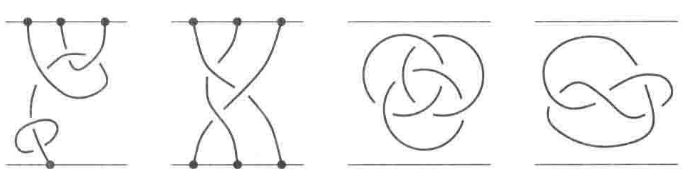


Figure 1 A tangle, a braid, a link, and a knot.

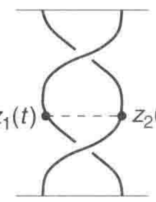


Figure 2 Counting the number of twists.

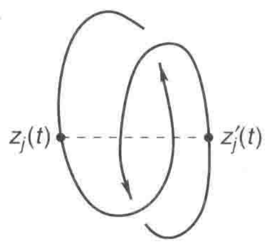


Figure 3 Counting the linking number.

Example 2 The linking number of two spatial curves K and K' (see **Figure 3**) can be computed as

$$\mathrm{lk}(K, K') = \frac{1}{2\pi \mathrm{i}} \int_{m<t<M} \sum_j \varepsilon_j \frac{\mathrm{d}(z_j(t) - z'_j(t))}{z_j(t) - z'_j(t)}$$

where m and M are the minimum and the maximum values of t on the link $K \cup K'$, j is the index that enumerates all possible choices of a pair of strands of the link as functions $z_j(t)$, $z'_j(t)$ corresponding to K and K', respectively, and $\varepsilon_j = \pm 1$ according to the parity of the number of chosen strands that are oriented downwards.

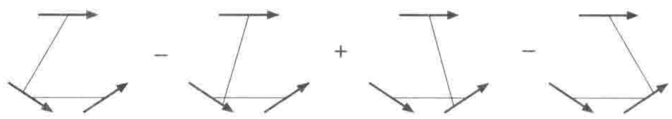
The Kontsevich integral can be regarded as a far-going generalization of these formulas. It aims at encoding all information about how the horizontal chords on the knot (or tangle) rotate when moved in the vertical direction. From a more general viewpoint, the Kontsevich integral represents the monodromy of the Knizhnik–Zamolodchikov connection in the complement to the union of diagonals in $\mathbb{C}^n$ (see Bar-Natan (1995a) and Ohtsuki (2002)).

Chord Diagrams and Weight Systems

Algebras $\mathcal{A}(p)$

The Kontsevich integral of a tangle T takes values in the space of chord diagrams supported on T.

Let X be an oriented one-dimensional manifold, that is, a collection of p numbered oriented lines and q numbered oriented circles. A chord diagram of order n supported on X is a collection of n pairs of unordered points in X, considered up to an orientation- and component-preserving diffeomorphism. In the vector space formally generated by all chord diagrams of order n, we distinguish the subspace spanned by all four-term relations



where thin lines designate chords, while thick lines are pieces of the manifold X. Apart from the fragments shown, all the four diagrams are identical. The quotient space over all such combinations is denoted by $\mathcal{A}_n(X) = \mathcal{A}_n(p, q)$. Let $\mathcal{A}(p, q) = \oplus_{n=0}^{\infty} \mathcal{A}_n(p, q)$ and let $\hat{\mathcal{A}}(p, q)$ be the graded completion of $\mathcal{A}(p, q)$ (i.e., the space of formal infinite series $\sum_{i=0}^{\infty} a_i$ with $a_i \in \mathcal{A}_i(p, q)$). If, moreover, we divide $\mathcal{A}(p, q)$ by all "framing independence" relations (any diagram with an isolated chord, i.e., a chord joining two adjacent points of the same connected component of X, is set to 0), then the resulting space is denoted by $\mathcal{A}'(p, q)$, and its graded completion by $\hat{\mathcal{A}}'(p, q)$.

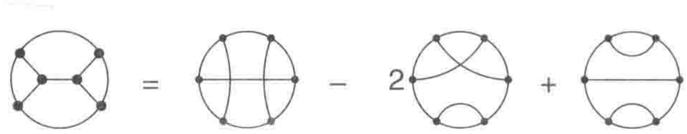
The spaces $\mathcal{A}(p, 0) = \mathcal{A}(p)$ have the structure of an algebra (the product of chord diagrams is defined by concatenation of underlying manifolds in agreement with the orientation). Closing a line component into a circle, we get a linear map $\mathcal{A}(p, q) \to \mathcal{A}(p-1, q+1)$ which is an isomorphism when $p = 1$. In particular, $\mathcal{A}(S^1) \cong \mathcal{A}(\mathbb{R}^1)$ has the structure of an algebra; this algebra is denoted simply by $\mathcal{A}$; the Kontsevich integral of knots takes its values in its graded completion $\hat{\mathcal{A}}$. Another algebra of special importance is $\hat{\mathcal{A}}(3) = \hat{\mathcal{A}}(3, 0)$, because it is where the Drinfeld associators live.

Hopf Algebra Structure

The algebra $\mathcal{A}(p)$ has a natural structure of a Hopf algebra with the coproduct δ defined by all ways to split the set of chords into two disjoint parts. To give a convenient description of its primitive space, one can use generalized chord diagrams. We now allow trivalent vertices not belonging to the supporting manifold and use STU relations (Bar-Natan 1995a)



to express the generalized diagrams as linear combinations of conventional chord diagrams, for example,



Then the primitive space coincides with the subspace of $\mathcal{A}(p)$ spanned by all connected generalized chord diagrams ("connected" means that they remain connected when the supporting manifold X is disregarded).

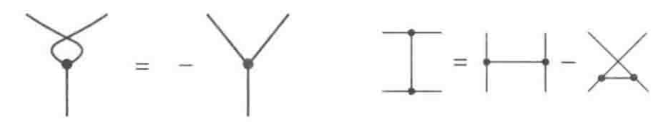
Weight Systems

A "weight system" of degree n is a linear function on the space $\mathcal{A}_n$. Every Vassiliev invariant v of degree n defines a weight system symb(v) of the same degree called its "symbol."

Algebras $\mathcal{B}(p)$

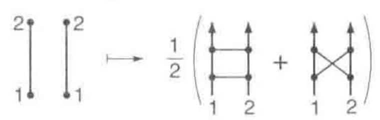
Apart from the spaces of chord diagrams modulo four-term relations, there are closely related spaces of Jacobi diagrams. A Jacobi diagram is defined as a unitrivalent graph, possibly disconnected, having at least one vertex of valency 1 in each connected component and supplied with two additional structures: a cyclic order of edges in each trivalent vertex and a labeling of univalent vertices taking values in the set $\{1, 2, \ldots, p\}$. The space $\mathcal{B}(p)$ is defined as the quotient of the vector space formally generated by all p-colored Jacobi diagrams modulo the two types of relations:

Antisymmetry: IHX:



The disjoint union of Jacobi diagrams makes the space $\mathcal{B}(p)$ into an algebra.

The symmetrization map $\chi_p: \mathcal{B}(p) \to \mathcal{A}(p)$, defined as the average over all ways to attach the legs of color i to ith connected component of the underlying manifold



is an isomorphism of vector spaces (the formal PBW isomorphism (Bar-Natan 1995a, Le and Murakami 1995) which is not compatible with the multiplication. The relation between $A(p)$ and $\mathcal{B}(p)$ very much resembles the relation between the universal enveloping algebra and the symmetric algebra of a Lie algebra. The algebra $\mathcal{B} = \mathcal{B}(1)$ is used to write out the explicit formula for the Kontsevich integral of the unknot (see Bar-Natan *et al.* (2003) and below).

The Construction

Kontsevich's Formula

We will explain the construction of the Kontsevich integral in the classical case of (closed) oriented knots; for an arbitrary tangle T, the formula is the same; only the result is interpreted as an element of $\hat{\mathcal{A}}(T)$. As above, represent three-dimensional space $\mathbb{R}^3$ as a direct product of a complex line $\mathbb{C}$ with coordinate z and a real line $\mathbb{R}$ with coordinate t. The integral is defined for Morse knots, that is, knots K embedded in $\mathbb{R}^3 = \mathbb{C}_z \times \mathbb{R}_t$ in such a way that the coordinate t restricted to K has only nondegenerate (quadratic) critical points. (In fact, this condition can be weakened, but the class of Morse knots is broad enough and convenient to work with.)

The Kontsevich integral $Z(K)$ of the knot K is the following element of the completed algebra $\hat{\mathcal{A}}'$:

$$Z(K) = \sum_{m=0}^{\infty} \frac{1}{(2\pi i)^m} \times \int_{\substack{t_{\min} < t_m < \cdots < t_1 < t_{\max} \\ t_j \text{ are noncritical}}} \sum_{P = \{(z_j, z'_j)\}} (-1)^{\downarrow_P} \times D_P \bigwedge_{j=1}^{m} \frac{dz_j - dz'_j}{z_j - z'_j}$$

Explanation of the Constituents

The real numbers $t_{\min}$ and $t_{\max}$ are the minimum and the maximum of the function t on K.

The integration domain is the m-dimensional simplex $t_{\min} < t_m < \cdots < t_1 < t_{\max}$ divided by the critical values into a certain number of "connected components." For example, **Figure 4** shows an embedding of the unknot where, for $m = 2$, the integration domain has six connected components.

The number of summands in the integrand is constant in each connected component of the integration domain, but can be different for different components. In each plane $\{t = t_j\} \subset \mathbb{R}^3$ choose an unordered pair of distinct points (z_j, t_j) and (z'_j, t_j) on K, so that $z_j(t_j)$ and $z'_j(t_j)$ are continuous branches of the knot. We denote by $P = \{(z_j, z'_j)\}$ the collection of such pairs for $j = 1, \ldots, m$. The integrand is the sum over all choices of the pairing P. In the example above for the component $\{t_{\min} < t_1 < c_1, c_2 < t_2 < t_{\max}\}$, we have only one possible pair of points on the levels $\{t = t_1\}$ and $\{t = t_2\}$. Therefore, the sum over P for this component consists of only one summand. Unlike this, in the component $\{t_{\min} < t_1 < c_1, c_1 < t_2 < c_2\}$, we still have only one

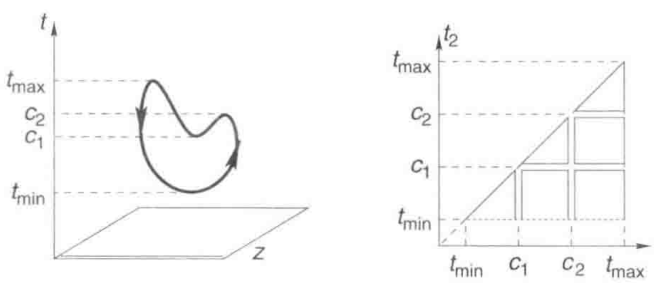


Figure 4 Connected components.

possibility for the level $\{t = t_1\}$, but the plane $\{t = t_2\}$ intersects our knot K in four points. So we have $\binom{4}{2} = 6$ possible pairs (z_2, z_2'), and the total number of summands is six (see **Figure 5**).

For a pairing P, the symbol "$\downarrow_P$" denotes the number of points (z_j, t_j) or (z_j', t_j) in P, where the coordinate t decreases along the orientation of K.

Fix a pairing P. Consider the knot K as an oriented circle and connect the points (z_j, t_j) and (z_j', t_j) by a chord. Up to a diffeomorphism, this chord does not depend on the value of t_j within a connected component. We obtain a chord diagram with m chords. The corresponding element of the algebra $\mathcal{A}'$ is denoted by D_P. **Figure 5**, for each connected component in our example, shows one of the possible pairings, the corresponding chord diagram with the sign $(-1)^{\downarrow}_P$ and the number of summands of the integrand (some of which are equal to zero in $\mathcal{A}'$ due to the framing independence relation).

Over each connected component, z_j and z_j' are smooth functions of t_j.

By

$$\bigwedge_{j=1}^{m} \frac{\mathrm{d}z_j - \mathrm{d}z_j'}{z_j - z_j'}$$

we mean the pullback of this form to the integration domain of variables $t_1, \ldots, t_m$. The integration domain is considered with the orientation of the space $\mathbb{R}^m$ defined by the natural order of the coordinates $t_1, \ldots, t_m$.

By convention, the term in the Kontsevich integral corresponding to $m = 0$ is the (only) chord diagram of order 0 with coefficient 1. It represents the unit of the algebra $\mathcal{A}'$.

Framed Version of the Kontsevich Integral

Let K be a framed oriented Morse knot with writhe number $w(K)$. Denote the corresponding knot without framing by $\bar{K}$. The framed version of the Kontsevich integral can be defined by the formula

$$Z^{\mathrm{fr}}(K) = \mathrm{e}^{(w(K)/2)\Theta} \cdot Z(\bar{K}) \in \hat{\mathcal{A}}$$

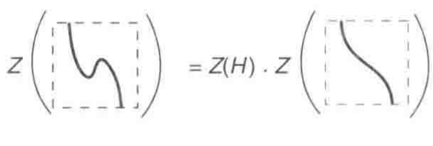
where Θ is the chord diagram with one chord and the integral $Z(\bar{K}) \in \hat{\mathcal{A}}'$ is understood as an element of the completed algebra $\hat{\mathcal{A}}$ (without one-term relations) by virtue of a natural inclusion $\mathcal{A}' \to \mathcal{A}$ defined as identity on the primitive subspace of $\mathcal{A}'$ (see Goryunov (1999) and Le and Murakami (1996)).

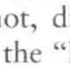
Basic Properties

Constructing the Universal Vassiliev Invariant

The Kontsevich integral $Z(K)$

1. converges for any Morse knot K,
2. is invariant under deformations of the knot in the class of Morse knots, and
3. behaves in a predictable way under the deformation that adds a pair of new critical points to a Morse knot:



Here the first and the third pictures depict two embeddings of an arbitrary knot, differing only in the shown fragment, $H =$  is the "hump" (unknot embedded in $\mathbb{R}^3$ in the specified way), and the product is the product in the completed algebra $\hat{\mathcal{A}}'$

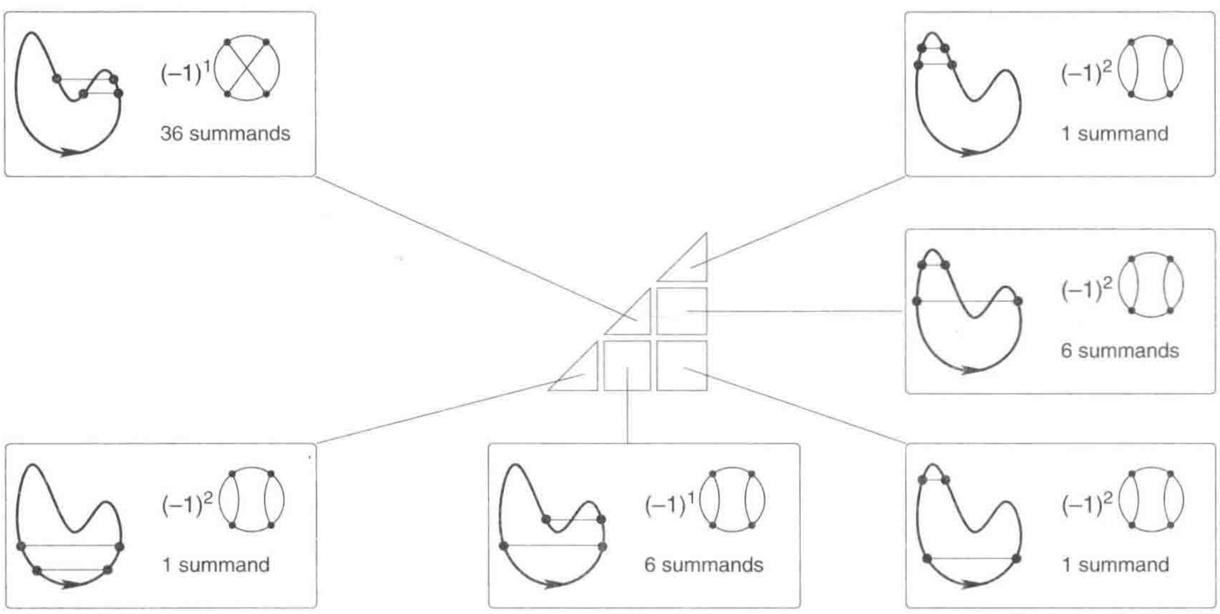


Figure 5 Pairings and chord diagrams.

of chord diagrams. The last equality allows one to define a genuine knot invariant by the formula

$$I(K) = Z(K)/Z(H)^{c/2}$$

where c denotes the number of critical points of K and the ratio means the division in the algebra $\hat{\mathcal{A}}'$ according to the rule $(1+a)^{-1} = 1 - a + a^2 - a^3 + \cdots$.

The expression $I(K)$ is sometimes referred to as the "final" Kontsevich integral as opposed to the "preliminary" Kontsevich integral $Z(K)$. It represents a universal Vassiliev invariant in the following sense: *Let w be a weight system, that is, a linear functional on the algebra $\hat{\mathcal{A}}'$. Then the composition $w(I(K))$ is a numerical Vassiliev invariant, and any Vassiliev invariant can be obtained in this way.*

The final Kontsevich integral for framed knots is defined in the same way, using the hump H with zero writhe number.

Is Universal Vassiliev Invariant Universal?

At present, it is not known whether the Kontsevich integral separates knots, or even if it can tell the orientation of a knot. However, the corresponding problem is solved, in the affirmative, in the case of braids and string links (theorem of Kohno–Bar-Natan (Bar-Natan 1995b, Kohno 1987).

Omitting Long Chords

We will state a technical lemma which is highly important in the study of the Kontsevich integral. It is used in the proof of the multiplicativity, in the combinatorial construction, etc.

Suppose we have a Morse knot K with a distinguished tangle T (**Figure 6**). Let m and M be the maximal and minimal values of t on the tangle T. In the horizontal planes between the levels m and M, we can distinguish two kinds of chords: "short" chords that lie either inside T or inside $K \setminus T$, and "long" chords that connect a point in T with a point in $K \setminus T$. Denote by $Z_T(K)$ the expression defined by the same formula as the Kontsevich integral $Z(K)$ where only short chords are taken into consideration. More exactly, if C is a connected component of the integration domain whose projection on the coordinate axis t_j is entirely contained in the segment $[m, M]$, then in the sum over the pairings P we include only those pairings that include short chords.

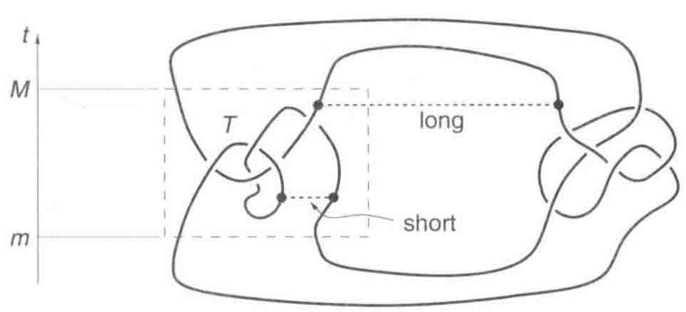


Figure 6 Short and long chords.

Lemma "Long" chords can be omitted when computing the Kontsevich integral: $Z_T(K) = Z(K)$.

Kontsevich's Integral and Operations on Knots

The Kontsevich integral behaves in a nice way with respect to the natural operations on knots, such as mirror reflection, changing the orientation of the knot, mutation of knots (see Chmutov and Duzhin (2001)), cabling (see Willerton (2002)). We give some details regarding the first two items.

Fact 1 Let R be the operation that sends a knot to its mirror image. Define the corresponding operation R on chord diagrams as multiplication by $(-1)^n$, where n is the order of the diagram. Then the Kontsevich integral commutes with the operation R: $Z(R(K)) = R(Z(K))$, where by $R(Z(K))$ we mean simultaneous application of R to all the chord diagrams participating in $Z(K)$.

Corollary *The Kontsevich integral $Z(K)$ and the universal Vassiliev invariant $I(K)$ of an amphicheiral knot K consist only of even order terms. (A knot K is called "amphicheiral," if it is equivalent to its mirror image: $K = R(K)$.)*

Fact 2 Let S be the operation on knots which inverts their orientation. The same letter will also denote the analogous operation on chord diagrams (inverting the orientation of the outer circle or, which is the same thing, axial symmetry of the diagram). Then the Kontsevich integral commutes with the operation S of inverting the orientation: $Z(S(K)) = S(Z(K))$.

Corollary *The following two assertions are equivalent:*

(i) *Vassiliev invariants do not distinguish the orientation of knots and*
(ii) *all chord diagrams are symmetric: $D = S(D)$ modulo four-term relations.*

The calculations of Kneissler (1997) show that up to order 12 all chord diagrams are symmetric. For bigger orders, the problem is still open.

Multiplicative Properties

The Kontsevich integral for tangles is multiplicative:

$$Z(T_1) \cdot Z(T_2) = Z(T_1 \cdot T_2)$$

whenever the product $T_1 \cdot T_2$, defined by vertical concatenation of tangles, exists. Here, the product

on the left-hand side is understood as the image of the element $Z(T_1) \otimes Z(T_2)$ under the natural map $\mathcal{A}(T_1) \otimes \mathcal{A}(T_2) \to \mathcal{A}(T_1 \cdot T_2)$.

This simple fact has two important corollaries:

1. For any knot K, the Kontsevich integral $Z(K)$ is a group-like element of the Hopf algebra $\hat{\mathcal{A}}'$, that is,
$$\delta(Z(K)) = Z(K) \otimes Z(K)$$
where δ is the comultiplication in $\mathcal{A}$ defined above.
2. The final Kontsevich integral, taken in a different normalization
$$I'(K) = Z(H)I(K) = \frac{Z(K)}{Z(H)^{c/2-1}}$$
is multiplicative with respect to the connected sum of knots:
$$I'(K_1 \# K_2) = I'(K_1)I'(K_2)$$

Arithmetical Properties

For any knot K the coefficients in the expansion of $Z(K)$ over an arbitrary basis consisting of chord diagrams are rational (see Kontsevich (1993), Le and Murakami (1996), and below).

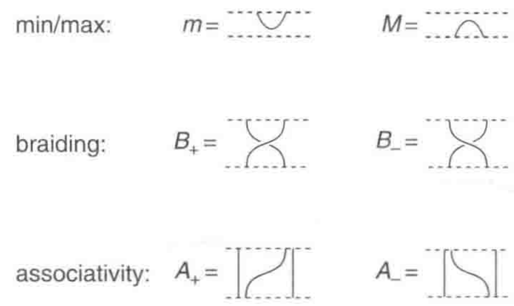
Combinatorial Construction of the Kontsevich Integral

Sliced Presentation of Knots

The idea is to cut the knot into a number of standard simple tangles, compute the Kontsevich integral for each of them, and then recover the integral of the whole knot from these simple pieces.

More exactly, we represent the knot by a family of plane diagrams continuously depending on a parameter $\varepsilon \in (0, \varepsilon_0)$ and cut by horizontal planes into a number of slices with the following properties.

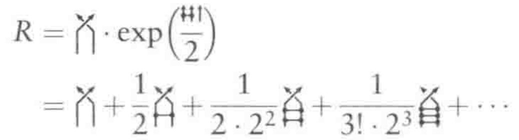
1. At every boundary level of a slice (dashed lines in the pictures below), the distances between various strings are asymptotically proportional to different whole powers of the parameter ε.
2. Every slice contains exactly one special event and several strictly vertical strings which are farther away (at lower powers of ε) from any string participating in the event than its width.
3. There are three types of special events:



where, in the two last cases, the strings may be replaced by bunches of parallel strings which are closer to each other than the width of this event.

Recipe of Computation of the Kontsevich Integral

Given such a sliced representation of a knot, the combinatorial algorithm to compute its Kontsevich integral consists in the following:

1. Replace each special event by a series of chord diagrams supported on the corresponding tangle according to the rule
$$m, M \mapsto 1$$
$$B_+ \mapsto R, \quad B_+ \mapsto R^{-1}$$
$$A_+ \mapsto \Phi, \quad A_- \mapsto \Phi^{-1}$$
where

$$\Phi = 1 - \frac{\zeta(2)}{(2\pi i)^2}[a, b] - \frac{\zeta(3)}{(2\pi i)^3}([a, [a, b]] + [b, [a, b]]) + \cdots$$
($\Phi \in \hat{\mathcal{A}}(3)$ is the Knizhnik–Zamolodchikov Drinfeld associator defined below; it is an infinite series in two variables $a =$ , $b =$ ).
2. Compute the product of all these series from top to bottom taking into account the connection of the strands of different tangles, thus obtaining an element of the algebra $\hat{\mathcal{A}}'$.

To accomplish the algorithm, we need two auxiliary operations on chord diagrams:

1. $S_i : \mathcal{A}(p) \to \mathcal{A}(p)$ defined as multiplication by $(-1)^k$ on a chord diagram containing k endpoints of chords on the string number i. This is the correction term in the computation of R and Φ in the case when the tangle contains

some strings oriented downwards (the upwards orientation is considered as positive).

2. $\Delta_i : \mathcal{A}(p) \to \mathcal{A}(p+1)$ acts on a chord diagram D by doubling the ith string of D and taking the sum over all possible lifts of the endpoints of chords of D from the ith string to one of the two new strings. The strings are counted by their bottom points from left to right. This operation can be used to express the combinatorial Kontsevich integral of a generalized associativity tangle (with strings replaced by bunches of strings) in terms of the combinatorial Kontsevich integral of a simple associativity tangle.

Example

Using the combinatorial algorithm, we compute the Kontsevich integral of the trefoil knot 3_1 to the terms of degree 2. A sliced presentation for this knot shown in **Figure 7** implies that $Z(3_1) = S_3(\Phi) R^{-3} S_3(\Phi^{-1})$ (here the product from left to right corresponds to the multiplication of tangles from top to bottom). Up to degree 2, we have

$$\begin{aligned}\Phi &= 1 + \tfrac{1}{24}[a,b] + \cdots \\ R &= X\left(1 + \tfrac{1}{2}a + \tfrac{1}{8}a^2 + \cdots\right)\end{aligned}$$

where X means that the two strands in each term of the series must be crossed over at the top. The operation S_3 changes the orientation of the third strand, which means that $S_3(a) = a$ and $S_3(b) = -b$. Therefore,

$$\begin{aligned}S_3(\Phi) &= 1 - \tfrac{1}{24}[a,b] + \cdots \\ S_3(\Phi^{-1}) &= 1 + \tfrac{1}{24}[a,b] + \cdots \\ R^{-3} &= X\left(1 - \tfrac{3}{2}a + \tfrac{9}{8}a^2 + \cdots\right)\end{aligned}$$

and

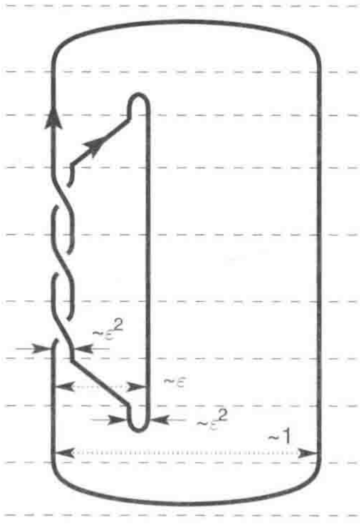


Figure 7 A sliced presentation of the trefoil.

$$\begin{aligned}Z(3_1) &= \left(1 - \tfrac{1}{24}[a,b] + \cdots\right) \\ &\quad \times X\left(1 - \tfrac{3}{2}a + \tfrac{9}{8}a^2 + \cdots\right)\left(1 + \tfrac{1}{24}[a,b] + \cdots\right) \\ &= 1 - \tfrac{3}{2}Xa - \tfrac{1}{24}abX + \tfrac{1}{24}baX \\ &\quad + \tfrac{1}{24}Xab - \tfrac{1}{24}Xba + \tfrac{9}{8}Xa^2 + \cdots\end{aligned}$$

Closing these diagrams into the circle, we see that in the algebra $\mathcal{A}$ we have $Xa = 0$ (by the framing independence relation), then $baX = Xab = 0$ (by the same relation, because these diagrams consist of two parallel chords) and $abX = Xba = Xa^2 = \otimes$. The result is $Z(3_1) = 1 + (25/24)\otimes + \cdots$. The final Kontsevich integral of the trefoil (in the multiplicative normalization) is thus equal to

$$\begin{aligned}I'(3_1) &= Z(3_1)/Z(H) \\ &= \left(1 + \frac{25}{24}\otimes + \cdots\right) \Big/ \left(1 + \frac{1}{24}\otimes + \cdots\right) \\ &= 1 + \otimes + \cdots\end{aligned}$$

Drinfeld Associator and Rationality

The Drinfeld associator used as a building block in the combinatorial construction of the Kontsevich integral can be defined as the limit

$$\Phi_{KZ} = \lim_{\varepsilon \to 0} \varepsilon^{-b} Z(AT_\varepsilon) \varepsilon^a$$

where $a =$ ⫲|, $b =$ |⫲, and AT_ε is the positive associativity tangle (special event A_+ shown above) with the distance between the vertical strands constant 1 and the distance between the close endpoints equal to ε. An explicit formula for Φ_{KZ} was found by Le and Murakami (1996); it is written as a nested summation over four variable multi-indices and therefore does not provide an immediate insight into the structure of the whole series; we confine ourselves by quoting the beginning of the series (note that Φ_{KZ} is a group-like element in the free associative algebra with two generators; hence, its logarithm belongs to the corresponding free Lie algebra):

$$\begin{aligned}\log(\Phi_{KZ}) = &-\zeta(2)[x,y] - \zeta(3)([x,[x,y]] + [y,[x,y]) \\ &- \frac{\zeta(2)^2}{10}(4[x,[x,[x,y]]] + [y,[x,[x,y]]] \\ &+ 4[y,[y,[x,y]]]) \\ &- \zeta(5)([x,[x,[x,[x,y]]]] + [y,[y,[y,[x,y]]]]) \\ &+ (\zeta(2)\zeta(3) - 2\zeta(5))([y,[x,[x,[x,y]]]] \\ &+ [y,[y,[x,[x,y]]]]) \\ &+ \left(\tfrac{1}{2}\zeta(2)\zeta(3) - \tfrac{1}{2}\zeta(5)\right)[[x,y],[x,[x,y]]] \\ &+ \left(\tfrac{1}{2}\zeta(2)\zeta(3) - \tfrac{3}{2}\zeta(5)\right)[[x,y],[y,[x,y]]] \\ &+ \cdots\end{aligned}$$

where $x = (1/2\pi i)a$ and $y = (1/2\pi i)b$. In general, Φ_{KZ} is an infinite series whose coefficients are "multiple zeta values" (Le and Murakami 1996, Zagier 1994)

$$\zeta(a_1, \dots, a_n) = \sum_{0<k_1<k_2<\cdots<k_n} k_1^{-a_1} \dots k_n^{-a_n}$$

There are other equivalent definitions of Φ_{KZ}, in particular one in terms of the asymptotical behavior of solutions of the simplest Knizhnik–Zamolodchikov equation

$$\frac{dG}{dz} = \left(\frac{a}{z} + \frac{b}{z-1}\right) G$$

where G is a function of a complex variable taking values in the algebra of series in two noncommuting variables a and b (see Drinfeld (1991)).

It turns out (theorem of Le and Murakami (1996)) that the combinatorial Kontsevich integral does not change if Φ_{KZ} is replaced by another series in $\hat{\mathcal{A}}(3)$ provided it satisfies certain axioms (among which the pentagon and hexagon relations are the most important, see Drinfeld (1991) and Le and Murakami (1996)).

Drinfeld (1991) proved the existence of an associator $\Phi_{\mathbb{Q}}$ with rational coefficients. Using it instead of Φ_{KZ} in the combinatorial construction, we obtain the following:

Theorem (Le and Murakami 1996). *The coefficients of the Kontsevich integral of any knot (tangle) are rational when $Z(K)$ is expanded over an arbitrary basis consisting of chord diagrams.*

Explicit Formulas for the Kontsevich Integral

The Wheels Formula

Let O be the unknot; the expression $I(O) = Z(H)^{-1}$ is referred to as the "Kontsevich integral of the unknot." A closed form formula for $I(O)$ was proved in Bar-Natan *et al.* (2003):

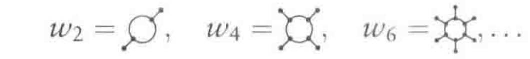
Theorem

$$I(O) = \exp \sum_{n=1}^{\infty} b_{2n} w_{2n} = 1 + \left(\sum_{n=1}^{\infty} b_{2n} w_{2n}\right) + \frac{1}{2}\left(\sum_{n=1}^{\infty} b_{2n} w_{2n}\right)^2 + \cdots$$

Here b_{2n} are modified Bernoulli numbers, that is, the coefficients of the Taylor series

$$\sum_{n=1}^{\infty} b_{2n} x^{2n} = \frac{1}{2} \ln \frac{e^{x/2} - e^{-x/2}}{x}$$

($b_2 = 1/48, b_4 = -1/5760, b_6 = 1/362\,880, \dots$), and w_{2n} are the "wheels," that is, Jacobi diagrams of the form



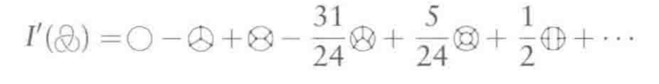
The sums and products are understood as operations in the algebra of Jacobi diagrams $\mathcal{B}$, and the result is then carried over to the algebra of chord diagrams $\mathcal{A}$ along the isomorphism χ.

Generalizations

There are several generalizations of the wheels formula.

1. Rozansky's rationality conjecture (Rozansky 2003) proved by Kricker (2000) affirms that the Kontsevich integral of any (framed) knot can be written in a form resembling the wheels formula. Let us call the "skeleton" of a Jacobi diagram the regular 3-valent graph obtained by "shaving off" all univalent vertices. Then the wheels formula says that all diagrams in the expansion of $I(O)$ have one and the same skeleton (circle), and the generating function for the coefficients of diagrams with n legs is a certain analytic function, more or less rational in e^x. In the same way, the theorem of Rozansky and Kricker states that the terms in $I(K) \in \hat{\mathcal{B}}$, when arranged by their skeleta, have the generating functions of the form $p(e^x)/A_K(e^x)$, where A_K is the Alexander polynomial of K and p is some polynomial function. Although this theorem does not give an explicit formula for $I(K)$, it provides a lot of information about the structure of this series.
2. Marché gives a closed form formula for the Kontsevich integral of torus knots $T(p, q)$.

The formula of Marché, although explicit, is rather intricate, and here, by way of example, we only write out the first several terms of the final Kontsevich integral I' for the trefoil (torus knot of type (2,3)), following Willerton (2002):



First Terms of the Kontsevich Integral

A Vassiliev invariant v of degree n is called "canonical" if it can be recovered from the Kontsevich integral by applying a homogeneous weight system, that is, if $v = \mathrm{symb}(v) \circ I$. Canonical invariants define a grading in the filtered space of Vassiliev invariants which is consistent with the filtration. If the Kontsevich integral is expanded

over a fixed basis in the space of chord diagrams $\hat{\mathcal{A}}'$, then the coefficient of every diagram is a canonical invariant. According to Stanford (2001) and Willerton (2002), the expansion of the final Kontsevich integral up to degree 4 can be written as follows:

$$\begin{aligned} I'(K) = \bigcirc & - c_2(K)\otimes - \tfrac{1}{6} j_3(K)\otimes \\ & + \tfrac{1}{48}(4j_4(K) + 36c_4(K) - 36c_2^2(K) + 3c_2(K))\otimes \\ & + \tfrac{1}{24}(-12c_4(K) + 6c_2^2(K) - c_2(K))\otimes \\ & + \tfrac{1}{2}c_2^2(K)\oplus + \cdots \end{aligned}$$

where c_n are coefficients of the Conway polynomial $\nabla_K(t) = \sum c_n(K)t^n$ and j_n are modified coefficients of the Jones polynomial $J_K(e^t) = \sum j_n(K)t^n$. Therefore, up to degree 4, the basic canonical Vassiliev invariants of unframed knots are c_2, j_3, j_4, $c_4 + (1/12)c_2$, and c_2^2.

Acknowledgments

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See also: Finite-Type Invariants; Mathematical Knot Theory.

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Korteweg–de Vries Equation and Other Modulation Equations

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Modulation equations are simplified equations used to model complicated physical systems. Typically they are derived from the fundamental partial differential equations that describe the system via asymptotic analysis. Furthermore, the modulation equations are in a sense "universal" in that many different physical systems are described by the same modulation equation. This comes about because the form of the modulation equation depends on only a very few, qualitative features of the original partial differential equation. Thus, they serve a sort of "normal form" for these partial differential equations and as such justify greater study than their apparently special character might otherwise merit.

The Korteweg–de Vries (KdV) equation

$$\partial_t u = \partial_x^3 u + 6u\partial_x u, \quad u = u(x,t), \ x \in \mathbf{R}, \ t \geq 0 \quad [1]$$

was one of the earliest modulation equations to be intensively studied. It was derived in an attempt to understand the propagation of solitary waves on the surface of water in a channel of finite depth. The KdV equation was first derived by Boussinesq but then independently rederived and studied in detail by Korteweg and de Vries. (For an interesting discussion of the early history of the KdV equation see Pego and Weinstein (1997).)

Derivation of the KdV Equation

As mentioned above, the KdV equation is a sort of normal form describing the propagation of small-amplitude, long-wavelength disturbances in a variety of different physical systems. In this section we describe in detail how it arises as an approximation to the Fermi–Pasta–Ulam (FPU) model of coupled, nonlinear oscillators. Although the KdV equation is most commonly encountered as an approximation to water waves, its study as an approximation to the FPU model was extremely important historically because it was in this context that its complete integrability was discovered by Miura (1968) and Gardner *et al.* (1974).

Consider an infinite set of particles of mass $m = 1$ at positions $q_j(t), j \in \mathbb{Z}$, interacting with their nearest neighbors via a potential $\mathcal{V}(q)$. Newton's equations for the motion of such particles are:

$$\frac{d^2 q_j}{dt^2} = \mathcal{V}'(q_{j+1}(t) - q_j(t)) - \mathcal{V}'(q_j(t) - q_{j-1}(t)), \quad j \in \mathbb{Z} \qquad [2]$$

If we rewrite these equations in terms of the difference variables $r(j,t) = q_{j+1}(t) - q_j(t)$, then [2] becomes

$$\frac{d^2 r}{dt^2}(j,t) = \mathcal{V}'(r(j+1,t)) + \mathcal{V}'(r(j-1,t)) - 2\mathcal{V}'(r(j,t)), \quad j \in \mathbb{Z} \qquad [3]$$

We are interested in small-amplitude, long-wavelength, solutions of [3]. One way of studying such motions is to change the lattice spacing in [3] from 1 to h and then let h tend to zero. A nice derivation of the KdV equation from that point of view is contained in Ablowitz and Segur (1981). Here, following Schneider and Wayne (1999), we will keep the lattice spacing fixed at 1 and rescale the spatial variable in the KdV equation. This is closer to the approximation method used in the water wave problem.

Since we want to focus on small-amplitude, long-wavelength solutions of [3], we begin by making the hypothesis that there exists some real-valued function $R(x,t)$ such that the solution of [3] can be written as

$$r(j,t) = \varepsilon^2 R(\varepsilon j, t) \qquad [4]$$

The prefactor ε^2 insures that the solution is of small amplitude while rescaling $j \to \varepsilon j$ means that phenomena that occur on length scales of $\mathcal{O}(1)$ in the equation for R will occur on length scales of $\mathcal{O}(1/\varepsilon)$ in the original equation – that is, they will be long-wavelength solutions. The differing powers of ε chosen for rescaling the amplitude and the spatial scale are chosen so that the dispersive and nonlinear effects will balance each other. Inserting [4] into [3] and expanding to lowest order in ε we find that the nonvanishing terms of lowest order in ε are

$$\frac{\partial^2 R}{\partial t^2} = \varepsilon^2 \mathcal{V}''(0) \frac{\partial^2 R}{\partial x^2} \qquad [5]$$

This is just the wave equation and thus to leading order we expect solutions of [3] to split into a left- and right-moving waves, each moving with speed $c_\varepsilon = \varepsilon\sqrt{\mathcal{V}''(0)}$. (We assume that $c^2 \equiv \mathcal{V}''(0) > 0$.) Thus, we make a refinement of the hypothesized form of the solution and replace [4] by

$$r(j,t) = \varepsilon^2 U(\varepsilon(j+ct), \varepsilon^3 t) + \varepsilon^2 V(\varepsilon(j-ct), \varepsilon^3 t) + \varepsilon^4 \varphi(\varepsilon j, \varepsilon t) \qquad [6]$$

The presence of the term $\varepsilon^4\varphi$ may be somewhat surprising. We will discuss the reason for its appearance in more detail below, but for the moment we mention merely that its presence does not affect the fact that to leading order the solution is approximated by the left- and right-moving waves represented by the $\varepsilon^2 U$ and $\varepsilon^2 V$ terms, respectively. We also note that the additional time dependence $\varepsilon^3 t$ in U and V is chosen, as is typical in the multiscale method to incorporate the higher-order terms omitted in [5] into the evolution.

Substituting [6] into [3] and expanding the resulting equation in ε we find that the lowest order in ε that occurs is $\mathcal{O}(\varepsilon^4)$ and these terms all cancel exactly because of the form of our hypothesized solution. The terms of $\mathcal{O}(\varepsilon^6)$ are:

$$\{2c\partial_X\partial_T U - 2c\partial_X\partial_T V + \partial_\tau^2\varphi\} = c^2\left(\tfrac{1}{12}\partial_X^4 U + \tfrac{1}{12}\partial_X^4 V + \partial_\xi^2\varphi\right) + \tfrac{1}{2}\mathcal{V}'''(0)\{\partial_X^2(U^2 + V^2 + 2UV)\} \qquad [7]$$

Here, X, T, ξ, and τ represent the rescaled independent variables, that is, $U = U(X,T), V = V(X,T)$, and $\varphi = \varphi(\xi,\tau)$.

Note that if it were not for the presence of the term $2UV$ on the right-hand side of this last equation the equations for U and V would completely decouple, that is, there would be no interaction between the left- and right-moving parts of the solution to this order. At this point, we can take advantage of the (heretofore) arbitrary function φ. If we assume that U and V are given, we can choose φ to satisfy the inhomogeneous wave equation:

$$\partial_\tau^2 \varphi = c^2 \partial_\xi^2 \varphi + \mathcal{V}'''(0) \partial_X^2 (UV) \quad [8]$$

Then, provided φ remains of $\mathcal{O}(1)$ over the timescales of interest (which one can verify *a posteriori*), we see that all terms of $\mathcal{O}(\varepsilon^6)$ in the expansion of [3] will vanish provided

$$\begin{aligned} 2\partial_T U &= \frac{c}{12} \partial_X^3 U + \frac{1}{2c} \mathcal{V}'''(0) \partial_X (U^2) \\ -2\partial_T V &= \frac{c}{12} \partial_X^3 V + \frac{1}{2c} \mathcal{V}'''(0) \partial_X (V^2) \end{aligned} \quad [9]$$

This means that the left- and right-moving parts of the solution satisfy a pair of uncoupled KdV equations.

Remark 1 To rewrite [9] in the standard form [1] one can make a simple rescaling – for instance, choose $X = \alpha x, T = t$ and $u(x,t) = \beta U(\alpha x, t)$, with $\alpha = (c/24)^{(1/3)}$ and $\beta = \mathcal{V}'''(0)/(12c\alpha)$.

We can now comment on the reasons we chose the particular scalings of the amplitude and of the independent variables used in [6]. The terms $\partial_X^2 U^2$ and $\partial_X^2 V^2$ are the lowest-order contributions from the nonlinear part of [3], while the terms $\partial_X^4 U$ and $\partial_X^4 V$ represent the lowest-order contributions from the linear part of the equation, except for the "trivial" translation that comes for [5]. In particular, in the absence of nonlinear effects the terms $\partial_X^4 U$ and $\partial_X^4 V$ (or equivalently, the terms $\partial_X^3 U$ and $\partial_X^3 V$ in [9]) would cause traveling waves to "disperse" and thus, the KdV equation represents a balance between nonlinear and dispersive effects. It is this balance between dispersion and nonlinearity which permits traveling-wave solutions to propagate without change of form (see the section "Integrability of the KdV equation").

More generally, we expect the KdV equation to arise as a modulation equation whenever a small-amplitude, long-wavelength linear wave is simultaneously perturbed by dispersive and nonlinear effects of the same order of magnitude. This is, of course, oversimplified. For instance, the original equation may have no quadratic terms in the nonlinearity, for instance, which means that the term $\partial_X U^2$ in the modulation equation will be replaced by a term like $\partial_X U^p$, for $p > 2$ – this leads to the modified KdV equation as the appropriate modulation equation. Or, for certain parameter values in the original equation the coefficient in front of the leading-order dispersive term may vanish, in which case a fifth-order modulation equation known as the Kawahara equation is more appropriate. However, both of these cases are in some sense nongeneric and the relatively weak hypotheses needed to obtain the KdV equation as the appropriate modulation equation indicate why it is encountered in so many diverse circumstances. We note, however, that the multiscale method used above to derive the KdV equation does not give a unique choice for the appropriate modulation equation at any given order of approximation and we discuss in a later section some other equations that could be used as models in the situation above.

Validity of the KdV Approximation

While the above derivation of the KdV equation is simple and intuitive one may wonder how accurate an approximation it actually provides to the true solutions of [3] (or to the evolution of water waves, probably the most important physical situation in which the KdV approximation is used). In particular, note that in the notation of [9] the phenomena intrinsic to the KdV equation occur on timescales $T = \mathcal{O}(1)$. However, this corresponds to a very long timescale $t = \mathcal{O}(1/\varepsilon^3)$ in the original FPU model and it could easily be the case that although the error made in derivation of the KdV approximation at any given time is quite small, over these very long timescales the errors could accumulate in such a way as to destroy the accuracy of the approximation.

The KdV and other modulation equations have been used since the nineteenth century but only relatively recently have rigorous estimates of the accuracy of this approximation been proved. In fact, the first estimates demonstrating that the KdV equation actually provided an accurate approximation to the true motion of water waves over the timescales expected from the heuristic derivation were not proved until Craig (1985). More recently, powerful general methods have been developed to justify not just the KdV equation but other modulation equations like the nonlinear Schrödinger equation and Ginzburg–Landau equation as well.

For instance, the following method, introduced in Kirrmann *et al.* (1992), has been used to justify the use of modulation equations in the water-wave problem, the evolution of Taylor–Couette patterns in viscous fluids, and a number of other

circumstances. We will explain it in the context of a general, abstract evolution equation to indicate its generality. Suppose that one wishes to approximate the small-amplitude solutions of a general evolution equation (or system of such equations) of the form

$$\partial_t u = Lu + \mathcal{N}(u) \qquad [10]$$

where L is a linear operator and $\mathcal{N}$ represents the nonlinear terms. Suppose that via some formal analysis like that in the previous section we have derived a function $\varepsilon^2\psi$ that is believed to be a good approximation to a true solution of [10]. In that example, for instance, $\varepsilon^2\psi$ would be the sum of the solutions of the two KdV equations in [9], and in general it will be given by the solution of the modulation equation that is expected to approximate [10]. We must show that the difference between $\varepsilon^2\psi$ and a true solution of [10] remains small over the timescales of interest. We write this difference as $u - \varepsilon^2\psi = \varepsilon^\beta R$ so that if $\beta > 2$, and if $R = \mathcal{O}(1)$, $\varepsilon^2\psi$ does provide the leading-order approximation to the true solution. We can make $R|_{t=0}$ small by choosing the initial conditions of our modulation equation appropriately and thus we need to follow how R evolves in time. If we use the equation satisfied by u we see that R evolves as

$$\begin{aligned}\partial_t R = LR + \varepsilon^{-\beta}[\mathcal{N}(\varepsilon^2\psi + \varepsilon^\beta R) \\ -\mathcal{N}(\varepsilon^2\psi)] + \varepsilon^{-\beta}\mathrm{Res}(\varepsilon^2\psi)\end{aligned} \qquad [11]$$

where $\mathrm{Res}(\varepsilon^2\psi) = L(\varepsilon^2\psi) + \mathcal{N}(\varepsilon^2\psi) - \partial_t(\varepsilon^2\psi)$, the "residual" of our approximation is simply the amount by which the approximation fails to satisfy the original equation at any given time. In the example in the previous section the residual would include the terms $\mathcal{O}(\varepsilon^8)$ that we ignored in our expansion.

One must now, in any given example consider three points:

1. The linear evolution of R:

$$\partial_t R = LR + D\mathcal{N}(\varepsilon^2\psi)R \qquad [12]$$

Controlling the solutions of this linear, but nonconstant coefficient partial differential equation is often the most difficult step in proving that solutions of the modulation equation give accurate approximations to the true solution. One can frequently find norms that are preserved by solutions of the leading-order equation $\partial_t R = LR$. However, the term $D\mathcal{N}(\varepsilon^2\psi) = \mathcal{O}(\varepsilon^2)$ if $\mathcal{N}$ is a quadratic nonlinearity. Over the very long timescales (i.e., $\mathcal{O}(\varepsilon^{-3})$) of interest in these approximation problems this $\mathcal{O}(\varepsilon^2)$ term can cause uncontrolled growth of R, leading to a breakdown in the approximation. In order to control [12] one must typically make use of some special features of the problem under consideration. For instance, it is sometimes possible to make a coordinate transformation which eliminates the terms of $\mathcal{O}(\varepsilon^2)$ on the right-hand side of [12], after which relatively standard methods suffice to control the solutions of [12].
2. The nonlinear terms in [11]: these terms are of the form $\varepsilon^{-\beta}[\mathcal{N}(\varepsilon^2\psi + \varepsilon^\beta R) - \mathcal{N}(\varepsilon^2\psi)] - D\mathcal{N}(\varepsilon^2\psi)R$. From Taylor's theorem we see that, if the nonlinear term is reasonably smooth, these terms are of $\mathcal{O}(\varepsilon^\beta)$. If $\beta > 3$, these terms are small and can be controlled over the timescales of interest by a straightforward application of Gronwall's inequality or standard "energy estimates."
3. Finally, one must consider the influence of the inhomogeneous terms $\varepsilon^{-\beta}\,\mathrm{Res}(\varepsilon^2\psi)$. Note that if this term is small enough, say $\mathcal{O}(\varepsilon^\beta)$, with $\beta \geq 3$ this term can also be controlled over the relevant timescales by an application of the Gronwall inequality. In order to make this term small, we need to be sure that our approximation $\varepsilon^2\psi$ fails to solve the true equation at any given time by a small amount. In doing so, we can exploit the fact that we can add to our leading-order approximation terms of higher order without affecting the fact that to leading order the true solution is still approximated by the solution of the modulation equation. This is the role of the term $\varepsilon^4\varphi$ in the approximation [6] in the previous section. The leading-order approximation is given by the functions U and V which solve the KdV equations but by adding the additional term $\varepsilon^4\varphi$ to the approximation we cancel the remaining terms of $\mathcal{O}(\varepsilon^6)$ in [7], thereby reducing the size of the residue in that example to $\mathcal{O}(\varepsilon^8)$. This method works in other examples as well so that the inhomogeneous term in [11] can usually be treated by this means. However, in each case, we must prove that the additional terms one adds to the approximation remain bounded over the timescales of interest and demonstrating this fact may not be as easy as it was in the case of the FPU model where the additional term satisfied a simple wave equation.

Using this approach one can show that the approximation derived heuristically in the previous section does accurately model the behavior of solutions of the FPU model over the expected timescales. More precisely, if $r(j, t)$ is the solution of [3] and if U and V are the solutions of the modulation equations [9] (with appropriately chosen, small-amplitude, long-wavelength initial

conditions), one can prove (see Schneider and Wayne (1999)) that for any $T_0 > 0$ there is an $\varepsilon_0 > 0$ and $C > 0$ such that for all $0 < \varepsilon < \varepsilon_0$,

$$\sup_{t\in[0,T_0/\varepsilon^3]} \|r(\cdot,t) - (\varepsilon^2 U(\varepsilon(\cdot + ct), \varepsilon^3 t) + (\varepsilon^2 V(\varepsilon(\cdot - ct), \varepsilon^3 t))\|_{\ell^\infty} \leq C\varepsilon^{7/2}$$

One can also use this method to show that the solution of the water-wave problem with general small-amplitude, long-wavelength, initial data can be approximated by the sum of the solutions of a pair of uncoupled KdV equations (Schneider and Wayne 2000), one representing the left-moving part of the solution and one representing the right-moving part of the solution, though in this context the technical difficulties associated with the existence theory for the water-wave problem mean the details are quite a lot more complicated.

Integrability of the KdV Equation

One reason that normal forms for systems of ordinary differential equations are so useful is that they are frequently integrable – that is, they possess sufficiently many integrals, or constants of motion, that essentially explicit formulas for their solutions can be obtained. Remarkably, the same is true for the KdV equation and for many other modulation equations. An argument for why this is so has been put forth by Calogero and Eckhaus based on the universality of these equations – see Calogero and Eckhaus (1987) and references therein, as well as the article Integrable Systems: Overview for more on this point.

Recall that Boussinesq and Korteweg and de Vries introduced the KdV equation to study solitary traveling waves on a fluid surface. For [1], one has an explicit family of such solutions given by:

$$u(x,t) = 2A^2 \mathrm{sech}^2(A[x + 4A^2 t]), \quad A \geq 0$$

Note that from this formula one sees that waves of large amplitude are narrower and travel faster than waves of small amplitude.

In a famous numerical study, Zabusky and Kruskal made a remarkable discovery. They considered solutions of the KdV equation in which a solitary wave of large amplitude overtook one of smaller amplitude. They found that after a highly nonlinear interaction the two solitary waves reemerged with their original amplitudes and speeds and the only reminder of their interaction was a phase shift in their relative positions. Their discovery began a search for a mathematical explanation of this remarkable "nonlinear superposition principle" which culminated with the solution of the KdV equation via the method of inverse scattering and the identification of the KdV equation as an infinite-dimensional, completely integrable Hamiltonian system.

We begin by describing how a transformation discovered by Miura (1968) and then generalized by Gardner *et al.* (1974) leads very easily to the conclusion that there are infinitely many conserved quantities for the KdV equation. The basic idea is that given a transformation which maps solutions of one equation to solutions of a second, the existence of simple or "obvious" conserved quantities for the first equation may lead, via the transformation, to more complicated conserved quantities for the second.

Given $u = u(x,t)$, define $w(x,t)$ implicitly via the formula

$$u(x,t) = w(x,t) + \mathrm{i}\varepsilon\partial_x w(x,y) + \varepsilon^2(w(x,t))^2 \quad [13]$$

Note that if w is smooth enough and ε is small, we can invert this relation recursively to obtain w in terms of u via the formula

$$\begin{aligned} w = u &- \mathrm{i}\varepsilon\partial_x u - \varepsilon^2(u^2 + \partial_x^2 u) \\ &+ \mathrm{i}\varepsilon^3(\partial_x^3 u + 4u\partial_x^2 u) + \varepsilon^4(2u^3 + 5(\partial_x u)^2 \\ &+ 6u\partial_x^2 u + \partial_x^4 u) + \mathcal{O}(\varepsilon^5) \end{aligned} \quad [14]$$

Now compute

$$\begin{aligned} &\partial_t u - \partial_x^3 u - 6u\partial_x u \\ &= \{\partial_t w - 6w\partial_x w - 6\varepsilon^2 w^2 \partial_x w - \partial_x^3 w\} \\ &\quad + 2\varepsilon^2 w\{\partial_t w - 6w\partial_x w - 6\varepsilon^2 w^2\partial_x w - \partial_x^3 w\} \\ &\quad + \mathrm{i}\varepsilon\partial_x\{\partial_t w - 6w\partial_x w - 6\varepsilon^2 w^2 \partial_x w - \partial_x^3 w\} \end{aligned} \quad [15]$$

From this we see immediately that if w satisfies the modified KdV equation

$$\partial_t w = 6(w\partial_x w + \varepsilon^2 w^2 \partial_x w) + \partial_x^3 w \quad [16]$$

then u, defined by [13] satisfies the KdV equation. However, one also sees immediately that the integral of w is a conserved quantity of [16] for all values of ε, that is, if we define $\mathcal{I}_\varepsilon(t) = \int w(x,t)\,\mathrm{d}x$, then $\mathcal{I}_\varepsilon$ is a constant for all values of ε. (We will assume here that w is defined on the real line, and that w and its derivatives go to zero as $|x|$ tends to infinity. Similar results hold for x running over a finite interval with periodic boundary conditions.) But this in turn immediately implies that if we use [14] to expand $\mathcal{I}_\varepsilon$ in powers of ε the coefficients in this expansion must also be constants in time. Since these coefficients will be expressed as integrals of u and its derivatives, they will give us (infinitely many)

conserved quantities for the KdV equation! Looking at the first few of these we find:

1. $K_0 = \int u(x,t)\,dx$. The conservation of this quantity follows immediately from the form of the KdV equation.
2. $K_1 = \int \partial_x u(x,t)\,dx = 0$, if we assume that u and its derivatives tend to zero as $|x|$ tends to infinity. Thus, we gain no new information from this quantity and in fact, all the integrals coming from the odd powers of ε turn out to be "trivial" so we ignore them and focus just on the even powers of ε.
3. $K_2 = \int (u^2 + \partial_x^2 u)\,dx = \int u^2\,dx$. That this is a conserved quantity is again easy to see directly from the KdV equation, just by multiplying the equation by u and integrating with respect to x.
4. $K_4 = \int (3u^2 + 5(\partial_x u)^2 + 6u\partial_x^2 u + \partial_x^4 u)\,dx = \int (3u^2 - (\partial_x u)^2)\,dx$. The origin of this integral is not so obvious and we comment further on its meaning below.

Clearly by continuing this procedure we can generate an infinite number of conserved quantities for the KdV equation. Indeed, if one chose another conserved quantity for the modified KdV equation, [16], say $\int w^2(x,t)\,dx$ one could generate another sequence of conserved quantities via this same procedure. However, Kruskal, Miura, Gardner, and Zabusky proved that in fact, all of the conserved quantities that can be written as polynomials in u and its derivatives are already obtained by the procedure above.

The constant of the motion K_4 found above is of particular interest because one can write the KdV equation as

$$u_t = \partial_x\left(\frac{\delta K_4}{\delta u}\right) \qquad [17]$$

where $\delta/\delta u$ denotes the variational derivative of K_4 with respect to $u(x)$. One can interpret this equation as a Hamiltonian system where ∂_x defines the (nonstandard) symplectic structure and remarkably, Zhakarov and Faddeev (1971) proved that the KdV equation is actually a completely integrable Hamiltonian system. In particular, there exists a canonical transformation such that with respect to the new coordinates the Hamiltonian is a function only of the action variables (and hence in particular, the action variables remain constant in time). The transform which brings the Hamiltonian into its action-angle form is known as the inverse spectral transform and its details would take us beyond the limits of this article. However, very briefly, by observing that the Miura transformation [13] defines a Ricatti differential equation, and using the transformation that converts the Ricatti equation to a linear ordinary differential equation one can relate the solution of the KdV equation to an eigenvalue problem for a linear Schrödinger operator. The potential term in the Schrödinger operator is given by the solution $u(x,t)$ of the KdV equation. Remarkably, it turns out that the eigenvalues of this Schrödinger operator are constants of the motion if u is a solution of the KdV equation and are very closely related to the action variables for the Hamiltonian system. For more details on the inverse-scattering method and its use in solving the KdV equation we refer the reader to the monographs of Ablowitz and Segur (1981), Newell (1985), or the recent book by Kappeler and Pöschel (2003) which develops the theory for the KdV equation on a finite interval with periodic boundary conditions in a particularly elegant fashion.

Other Mathematical Aspects of the KdV Equation

In addition to the inverse-scattering transform approach, more traditional approaches to the existence and uniqueness of solutions have also been studied, starting with Temam's proof of the well-posedness of solutions of the KdV equation with periodic boundary conditions in the Sobolev space H^2. Noting that the Hamiltonian for the KdV equation described in the preceding section is closely related to the H^1 norm, this might seem a natural space in which to study well-posedness, but surprisingly Kenig, Ponce, and Vega, and Bourgain showed that the equation is also well posed in Sobolev spaces H^s, with $s < 1$ and more recent work has extended the global well-posedness results to Sobolev spaces of small negative order. Aside from their intrinsic interest, these results have other physical implications. If one wishes to study statistical aspects of the behavior of ensembles of solutions of these equations, statistical mechanics suggests that the natural invariant measure for these equations is given by the Gibbs' measure. However, the Gibbs' measure is typically supported on functions less regular than H^1, so that in order to define and study this measure one needs to know that solutions of the equation are well behaved in such spaces.

Another natural mathematical question arises from the fact that the KdV equation is only an approximation to the original physical equation. Viewed from another perspective, the original system can be seen as a perturbation of the KdV equation. It then becomes natural to ask whether the special features of the KdV equation are preserved under perturbation. Viewing the KdV equation as a completely integrable Hamiltonian system this is

very analogous to the questions studied by the Kolmogorov–Arnol'd–Moser (KAM) theory and has led to a development of KAM-like results for a number of different partial differential equations like the KdV equation. The results are somewhat technical in nature but roughly speaking they say that if one considers the KdV equation with periodic boundary conditions, temporally periodic or quasi-periodic solutions will persist under small perturbations. The situation is more complicated and less well understood for the equation on the whole line due to the presence of a continuum of scattering states. For a very thorough review of the problem with periodic boundary conditions see Kappeler and Pöschel (2003).

Other Modulation Equations

As we stressed in its derivation, the KdV equation is an appropriate modulation equation for small-amplitude, long-wavelength solutions in dispersive nonlinear partial differential equations. However, as mentioned in the section "Derivation of the KdV equation" the method of multiple scales does not give a unique modulation equation even in this specific physical regime. Already in his original studies Boussinesq derived at least three different model equations for small-amplitude, long-wavelength water waves and a variety of such models continue to be studied today. For instance, an easy variation in the derivation of the KdV equation leads to the regularized long wave, or Benjamin–Bona–Mahoney equation in which the $\partial_x^3 u$ term in the KdV equation is replaced by the term $\partial_x^2 \partial_t u$. The validity of these alternatives to the KdV equation can also be studied with the aid of the methods described in the section "Validity of the Kdv approximation."

There have been many discussions of which of these modulation equations is the "correct" one. while they may all yield equivalent approximations to the original physical problem the KdV equation has at least two advantages: it is independent of the expansion parameter ε, and it is completely integrable. None of the other equations that have been proposed as approximations to these small-amplitude, long-wavelength phenomena share both of these properties.

If we think in terms of the Fourier transforms of the long-wavelength functions studied above they are solutions whose Fourier transform is concentrated near zero. One can also ask about modulation equations for solutions whose Fourier transform is concentrated about nonzero wave numbers. Such solutions represent a wave train with some fixed underlying wavelength, λ_c, modulated on a much longer length scale, λ_c/ε.

If we make the ansatz that the solution has the form

$$u(x,t) \approx \varepsilon A(\varepsilon(x - c_g t), \varepsilon^2 t) e^{i2\pi(x - c_p t)/\lambda_c} + \text{complex conjugate} \qquad [18]$$

and insert this hypothesized form of the solution into the original equation, then under mild assumptions on the form and properties of the original equation, similar to those under which we derived the KdV equation in an earlier section we find that to the lowest, nontrivial order in ε, the amplitude A evolves according to the nonlinear Schrödinger equation

$$-i\partial_T A = c_1 \partial_X^2 A + c_2 A|A|^2 \qquad [19]$$

If c_1 and c_2 are both real, the nonlinear Schrödinger equation can also be solved via the inverse-scattering method and it represents another completely integrable modulation equation.

In this article, we have discussed modulation equations only for Hamiltonian, or conservative systems. However, similar equations have also played an important role in the study of dissipative equations like the Navier–Stokes equation. The most common modulation context in that setting is the Ginzburg–Landau equation, which can be derived as a modulation equation for Taylor–Couette rolls or for the convection rolls in the Rayleigh–Bénard problem. Like the nonlinear Schrödinger equation, the Ginzburg–Landau equation describes how slow variations of the amplitude of an underlying periodic pattern evolve and as such it arises in a host of other situations in addition to the fluid dynamics examples mentioned above. For an extensive review of the applications of the Ginzburg–Landau equation, as well as its mathematical properties and some special solutions, see the recent article of Mielke (2002).

See also: Bi-Hamiltonian Methods in Soliton Theory; Central Manifolds, Normal Forms; Hamiltonian Fluid Dynamics; Infinite-Dimensional Hamiltonian Systems; Integrable Systems and the Inverse Scattering Method; Integrable Systems: Overview; KAM Theory and Celestial Mechanics; Multiscale Approaches; Partial Differential Equations: Some Examples; WDVV Equations and Frobenius manifolds.

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K-Theory

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K-theory was invented in the category of algebraic vector bundles over algebraic varieties by A Grothendieck, who was directly motivated by the Hirzebruch–Riemann–Roch theorem which he subsequently greatly generalized. He also defined *K*-homology in terms of coherent sheaves and established the basic properties of *K*-theory and *K*-homology including Poincaré duality for nonsingular varieties. The origin for the choice of the letter *K* in *K*-theory was apparently the German word "Klasse."

Using the formalism of Grothendieck, M F Atiyah and F Hirzebruch (cf. Karoubi 1978), developed topological *K*-theory in the category of topological (complex) vector bundles over topological spaces. It is this theory that will be the first principal focus of this article. A topological (complex) vector bundle over a compact topological space X is a topological space E together with a continuous map $p: E \to X$ that is onto, such that $p^{-1}(x)$ is a vector space that is isomorphic to $\mathbb{C}^n$ for all $x \in X$, and there is an open cover $\{U\}$ of X together with homeomorphisms $h_U: p^{-1}(U) \to U \times \mathbb{C}^n$ called "local trivializations" with the property that $h_V \circ h_U^{-1}: U \cap V \times \mathbb{C}^n \to U \cap V \times \mathbb{C}^n$ is of the form (Id, g_{UV}), where $g_{UV}: U \cap V \to \mathrm{GL}(n, \mathbb{C})$ are continuous maps satisfying the following cocycle condition on triple overlaps, $g_{UV} g_{VW} g_{WU} = 1$. $X \times \mathbb{C}^n$ is called the trivial vector bundle. Two vector bundles $p: E \to X$ and $q: F \to X$ over X are said to be isomorphic if there is a homeomorphism $\phi: E \to F$ with the property that $p = q \circ \phi$, and which is a linear isomorphism when restricted to each fiber. The direct sum and tensor product of vector spaces carries over to vector bundles. There are canonical isomorphisms $E \oplus F \cong F \oplus E$ and $E \otimes F \cong F \otimes E$, making the set $\mathrm{Vect}(X)$ of isomorphism classes of complex vector bundles over X into a commutative semiring. $\mathrm{Vect}(X)$ can be made into the commutative ring $K^0(X)$ as follows. $K^0(X)$ is generated by pairs $([E], [F])$, together with the relation $([E], [F]) = ([E'], [F'])$ if $E \oplus F' \oplus G \cong E' \oplus F \oplus G$ for some $[G] \in \mathrm{Vect}(X)$. Also $K^1(X)$ is defined to be the group of homotopy classes of continuous maps from X to the infinite unitary group. Around the same time, R Bott proved his celebrated periodicity theorem, which says that the odd homotopy group of the (infinite) unitary group is the integers, whereas the even homotopy groups are all trivial. Incorporating Bott's periodicity theorem for the unitary group into *K*-theory, Atiyah and Hirzebruch proved that topological *K*-theory $K^\bullet(X) = K^0(X) \oplus K^1(X)$ is a periodic generalized cohomology theory, and in what follows, the notation $K^n(X)$ means n modulo 2. If M is not compact, then we can compactify M by adding to it a point $+$ "at infinity," and denote it by M^+. Let $\iota: + \to M^+$ be the inclusion, inducing the pullback

map $\iota^!: K^\bullet(M^+) \to K^\bullet(+) \cong \mathbb{Z}$. Then $K^\bullet(M)$ is defined to be $\ker(\iota^!)$, also called the reduced K-theory. If X_1 is a closed subset of X, the K-theory of the pair (X, X_1) is defined as the reduced K-theory of the quotient space X/X_1. A fundamental computation of Bott is the computation of the K-theory of Euclidean space, $K^n(\mathbb{R}^n) \cong \mathbb{Z}$ with canonical generator called the Bott class $b \in K^n(\mathbb{R}^n)$, and $K^{n-1}(\mathbb{R}^n) = \{0\}$.

Some of the basic properties of K-theory are listed as follows. Details can be found in Karoubi (1978).

1. *Pullback* If $f: N \to M$ is a continuous map, then given a vector bundle $\pi: E \to M$ over M, the pullback vector bundle is defined as $f^*(E) = \{(x, v) \in N \times E : f(x) = \pi(v)\}$ over N. This induces a pullback homomorphism, $f^!: K^\bullet(M) \to K^\bullet(N)$.
2. *Push-forward* Let $f: N \to M$ be a smooth proper map between compact manifolds which is K-oriented, that is, $TN \oplus f^*TM$ is a spin$^{\mathbb{C}}$ vector bundle over N. Then there is a pushforward homomorphism, also called a Gysin map, $f_!: K^\bullet(N) \to K^{\bullet+d}(M)$. where $d = \dim M - \dim N$, whose construction will be explained in the next section.
3. *Homotopy* If $f: N \to M$ and $g: N \to M$ are homotopic maps, then the pullback maps $f^! = g^!$ are equal. If in addition, f and g are K-oriented, proper maps which are homotopic via proper maps, then the Gysin maps $f_! = g_!$ are equal.
4. *Excision* Let M_1 be a closed subset of M and U be an open subset of M such that U is contained in the interior of M_1. Then the inclusion of pairs $(M \setminus U, M_1 \setminus U) \hookrightarrow (M, M_1)$ induces an isomorphism in K-theory, $K^\bullet(M, M_1) \cong K^\bullet(M \setminus U, M_1 \setminus U)$.
5. *Exactness* Let M_1 be a closed subset of M. Then there is a six-term exact sequence in K-theory,

$$\begin{array}{ccccc} K^0(M, M_1) & \longrightarrow & K^0(M) & \longrightarrow & K^0(M_1) \\ \uparrow & & & & \downarrow\Delta \\ K^1(M_1) & \longleftarrow & K^1(M) & \longleftarrow & K^1(M, M_1) \end{array}$$

6. *Cup product* There is a canonical map given by external tensor product, $K^i(M) \otimes K^j(N) \to K^{i+j}(M \times N)$. When $N = M$, one can compose this with the homomorphism induced by the diagonal map $M \to M \times M$ given by $x \to (x, x)$, to get a cup product, $K^p(M) \otimes K^q(M) \to K^{p+q}(M)$.
7. *Bott periodicity* This is arguably the most important property of K-theory. It says that the zero-section embedding $\iota^M: M \hookrightarrow M \times \mathbb{R}^n$ induces a Gysin isomorphism, $\iota^M{}_!: K^\bullet(M) \xrightarrow{\cong} K^{\bullet+n}(M \times \mathbb{R}^n)$, which is given as follows. Let $\pi_M: M \times \mathbb{R}^n \to M$ and $\pi_{\mathbb{R}^n}: M \times \mathbb{R}^n \to \mathbb{R}^n$ denote the projections onto the factors, and $b = \iota_! 1 \in K^n(\mathbb{R}^n)$ the Bott element, where $\iota: \{0\} \hookrightarrow \mathbb{R}^n$ is the inclusion of the origin. Then the Bott periodicity isomorphism is given by $\iota^M{}_!(x) = \pi^!_M(x) \cup \pi^!_{\mathbb{R}^n}(b) \in K^{\bullet+n}(M \times \mathbb{R}^n)$ for all $x \in K^\bullet(M)$.

Using the fact that any vector bundle over a contractible space is trivial, together with Bott's periodicity theorem, one deduces the calculation of the K-theory of spheres. The calculation for the odd-dimensional spheres given, $K^0(S^{2n-1}) \cong \mathbb{Z} \cong K^1(S^{2n-1})$, and for the even-dimensional spheres $K^0(S^{2n-1}) \cong \mathbb{Z}^2$ and $K^1(S^{2n}) \cong \{0\}$, for all $n \geq 1$.

There is a natural homomorphism of rings called the Chern character, $\mathrm{Ch}: K^\bullet(X) \to H^\bullet(X, \mathbb{Q})$ which is characterized by the following axioms:

1. *Naturality* If $f: N \to M$ is a smooth map, and if E is a vector bundle over M, then $\mathrm{Ch}(f^!(E)) = f^*(\mathrm{Ch}(E))$.
2. *Additivity* $\mathrm{Ch}(E \oplus F) = \mathrm{Ch}(E) + \mathrm{Ch}(F)$.
3. *Normalization* If L is the canonical line bundle over $\mathbb{C}P^n$ which restricts to the Hopf line bundle over $\mathbb{C}P^1$, then $\mathrm{Ch}(L) = \exp(x)$, where x is the generator of $H^2(\mathbb{C}P^n, \mathbb{Z}) \cong \mathbb{Z}$.

Atiyah and Hirzebruch, cf. Karoubi (1978), also proved that the Chern character induces an isomorphism of the rings $K^\bullet(X) \otimes \mathbb{Q}$ and $H^\bullet(X, \mathbb{Q})$. The Chern–Weil representative of the Chern character is $\mathrm{tr}(\exp((\mathrm{i}/2\pi)\Omega_E))$, where Ω_E is the curvature of a Hermitian connection on E.

There are many variants of K-theory, such as KO-theory, where the unitary group is replaced by the orthogonal group, which is periodic of order eight, and G-equivariant K-theory, where G is a compact Lie group. K-theory and its variants have many interesting applications such as determining the maximum number of linearly independent vector fields on spheres, which is due to Adams, cf. Karoubi (1978). We will content ourselves with the description of two important applications.

Grothendieck–Riemann–Roch Theorem for Smooth Manifolds

Recall that an oriented real vector bundle E over M is said to be a spin$^{\mathbb{C}}$ vector bundle if the bundle of oriented frames on E, $\mathrm{SO}(E)$ has a circle bundle $\mathrm{Spin}^{\mathbb{C}}(E)$ such that the restriction to each fiber yields the central extension $0 \to \mathrm{U}(1) \to \mathrm{Spin}^{\mathbb{C}}(n) \to \mathrm{SO}(n) \to 0$ that defines the group $\mathrm{Spin}^{\mathbb{C}}(n)$, where n is the rank of E. It turns out that the obstruction to the existence of a spin$^{\mathbb{C}}$ structure on E is the third integral Stieffel–Whitney class of E, $W_3(E) \in H^3(M, \mathbb{Z})$.

A generalization of Bott periodicity is the Thom isomorphism in K-theory. It says that if $\pi: E \to M$ is a rank-n spin$^{\mathbb{C}}$ vector bundle over M, then the zero-section embedding $\iota^M: M \hookrightarrow E$ induces a Gysin isomorphism, $\iota^M{}_!: K^\bullet(M) \cong K^{\bullet+n}(E)$, which is given as follows. There is a canonical element $\iota_!^M 1 \in K^n(E)$ called the Thom class in K-theory, which is characterized by the property that $\iota_! 1$ restricts to give the Bott class on each fiber. Then the Thom isomorphism in K-theory is given by $\iota^M{}_!(x) = \pi^!(x) \cup \iota_!^M 1 \in K^{\bullet+n}(E)$ for all $x \in K^\bullet(M)$. For canonical representatives of the Thom class, cf. Mathai–Quillen Formalism, or Mathai and Quillen (1986).

Recall the definition of the Gysin map for smooth embeddings. Let X be a smooth, compact manifold, and Y a smooth manifold. Let $h: X \to Y$ be a smooth embedding that is K-oriented. Since $TX \oplus TX$ has a canonical almost-complex structure, it follows that the normal bundle $N_Y X = h^*(TY)/TX$ is a spin$\mathbb{C}$ vector bundle. If $\iota^X: X \hookrightarrow N_Y X$ is the zero-section embedding, then we have the Thom isomorphism $\iota_!^X: K^\bullet(X) \stackrel{\cong}{\to} K^{\bullet+n}(N_Y X)$, where $n = \dim(Y) - \dim(X)$ is the codimension of the embedding. Upon choosing a Riemannian metric on Y, there is a diffeomorphism Φ from a tubular neighborhood U of $h(X)$ onto a neighborhood of the zero section in the normal bundle $\iota(X)$. That is, $\Phi^!: K^\bullet(N_Y X) \stackrel{\cong}{\to} K^\bullet(U)$. For any open subset $j: U \hookrightarrow Y$, the extension by zero defines a homomorphism $j: K^\bullet(U) \to K^\bullet(Y)$. Then the Gysin map of the embedding h is defined as $h_! = j \circ \Phi^! \circ \iota_!^X: K^\bullet(X) \to K^{\bullet+n}(Y)$, which turns out to be independent of the choices made.

Next recall the definition of the Gysin map for smooth submersions. Let $\pi: Y \to Z$ be a smooth submersion of smooth manifolds, which is K-oriented and a proper map. Since every smooth compact manifold can be smoothly embedded in $\mathbb{R}^{2q}$ for q sufficiently large, a parametrized version yields an embedding $\kappa: Y \hookrightarrow Z \times \mathbb{R}^{2q}$ that is spin$\mathbb{C}$. Therefore the Gysin map is a homomorphism $\kappa_!: K^\bullet(Y) \to K^{\bullet+a}(Z \times \mathbb{R}^{2q})$, where $a = \dim(Z) + 2q - \dim(Y)$. Let $\iota^Z: Z \hookrightarrow Z \times \mathbb{R}^{2q}$ denote the zero-section embedding. Then we have the Thom isomorphism $\iota_!^Z: K^\bullet(Z) \stackrel{\cong}{\to} K^{\bullet+2q}(Z \times \mathbb{R}^{2q})$. Then the Gysin map of the submersion π is defined as $\pi_! = \kappa_! \circ (\iota_!^Z)^{-1}$: $K^\bullet(Y) \to K^{+b}(Z)$, where $b = \dim(Y) - \dim(Z)$, and turns out to be independent of the choices made.

Let $f: N \to M$ be a smooth proper map that is K-oriented. Then f can be canonically factored, first into the smooth embedding $\mathrm{gr}(f): N \hookrightarrow N \times M$, which is the graph of the function, that is, $\mathrm{gr}(f)(x) = (x, f(x))$, and which is K-oriented. The Gysin map is $\mathrm{gr}(f)_!: K^\bullet(N) \to K^{\bullet+\dim(M)}(N \times M)$. Second, the projection $p_M: N \times M \to M$ is a K-oriented proper submersion, when restricted to the image of $\mathrm{gr}(f)$. The Gysin map is $p_{M!}: K^\bullet(M \times N) \to K^{\bullet+b}(M)$, where $b = \dim(N)$. The Gysin map of f is defined as $f_! = p_{M!} \circ \mathrm{gr}(f)_!: K^\bullet(N) \to K^{\bullet+d}(M)$, where $d = \dim(M) + \dim(N)$.

Given such a smooth proper map $f: N \to M$ that is K-oriented. Then there are Gysin maps in cohomology, $f_*: H^\bullet(N, \mathbb{Q}) \to H^{\bullet+d}(M, \mathbb{Q})$ (where we consider the $\mathbb{Z}_2$-grading given by even and odd degree), and in K-theory, $f_!: K^\bullet(N) \to K^{\bullet+d}(M)$ which increases the degree by $d = \dim(M) + \dim(N)$. The Grothendieck–Riemann–Roch theorem due to Atiyah and Hirzebruch, cf. Karoubi 1978, in the smooth category can be phrased as the commutativity of the diagram,

$$\begin{array}{ccc} K^\bullet(N) & \stackrel{f_!}{\longrightarrow} & K^{\bullet+d}(M) \\ {\scriptstyle \mathrm{Todd}(TN)\cup \mathrm{Ch}}\downarrow & & \downarrow{\scriptstyle \mathrm{Todd}(TM)\cup \mathrm{Ch}} \\ H^\bullet(N, \mathbb{Q}) & \stackrel{f_*}{\longrightarrow} & H^{\bullet+d}(M, \mathbb{Q}) \end{array}$$

That is,

$$\mathrm{Ch}(f_!(\xi)) \cup \mathrm{Todd}(TM) = f_*(\mathrm{Ch}(\xi) \cup \mathrm{Todd}(TN))$$

for all $\xi \in K^\bullet(N)$, where $\mathrm{Todd}(E)$ is the Todd genus characteristic class of a Hermitian vector bundle E over M. The Chern–Weil representative of the Todd genus is

$$\sqrt{\det\left(\frac{(i/2\pi)\Omega_E}{\tanh((i/2\pi)\Omega_E)}\right)}$$

where Ω_E is the curvature of a Hermitian connection on E. There are many useful variants of this beautiful formula.

The Atiyah–Singer Index Theorem

The 2004 Abel Prize citation mentions the Atiyah–Singer (1971) index theorem as being one of the greatest achievements of twentieth-century mathematics. It has stimulated considerable interaction between mathematicians and mathematical physicists. We content ourselves here with a rudimentary description of the results.

Let $\mathcal{F}$ be the space of all Fredholm operators on an infinite-dimensional complex Hilbert space $\mathcal{H}$. Recall that an operator A is said to be Fredholm if both the kernel and cokernel of A are finite dimensional. The index of such a Fredholm operator is $\mathrm{index}(A) = \dim(\ker(A)) - \dim(\mathrm{coker}(A)) \in \mathbb{Z}$. The index map is continuous, so it induces a map on the connected components of $\mathcal{F}$, which turns out to be an isomorphism.

K-theory is naturally related to the space of all Fredholm operators $\mathcal{F}$ endowed with the norm topology. Any continuous map $A : X \to \mathcal{F}$ from a compact space to $\mathcal{F}$ has an index in $K^0(X)$, which is given by $\text{index}(A) = \ker(A) - \text{coker}(A)$ in the special case when $\dim(\ker(A))(x)$ is constant in $x \in X$. In general, one uses the fact that the index is stable under compact perturbation, and shows that one can always achieve the special case after a compact perturbation. It is again the case that the index map is continuous, and so induces a map, $\text{index}: [X, \mathcal{F}] \to K^0(X)$, which turns out to be an isomorphism, thanks to a fundamental theorem of Kuiper which proves that the group of all invertible operators on an infinite-dimensional complex Hilbert space is contractible in the norm topology.

Now let $\pi : N \to Z$ be a fiber bundle with typical fiber a smooth compact manifold M, where N and Z are also smooth compact manifolds. Consider a smooth family of elliptic operators $D = \{D_z\}_{z \in Z}$ along the fibers of π, parametrized by Z, where $D_z : C^\infty(\pi^{-1}(z), E|_{\pi^{-1}(z)}) \to C^\infty(\pi^{-1}(z), F|_{\pi^{-1}(z)})$ and E, F are vector bundles over N. Such a family of elliptic operators has a symbol

$$\sigma(D) : \pi^*(E) \to \pi^*(F)$$

where $\pi : T^*(N/Z) \to N$ is the projection and $T^*(N/Z)$ is the vertical cotangent bundle. Ellipticity for the family is the condition that $\sigma(D)$ is an isomorphism outside the zero section, so that the triple $(\pi^*(E), \pi^*(F), \sigma(D))$ determines an element in $K^0(T^*(N/Z))$ denoted by $\sigma(D)$.

The analytic index of the family D is $\text{index}(D) \in K^0(Z)$, and it turns out that it only depends on the class of the symbol $\sigma(D) \in K^0(T^*(N/Z))$, so the analytic index can be viewed as a homomorphism,

$$\text{index} : K^0(T^*(N/Z)) \to K^0(Z)$$

Consider an embedding $\iota : N \hookrightarrow Z \times \mathbb{R}^n$ that is compatible with the projection $\pi : N \to Z$. The fiberwise differential is an embedding $d\iota : T(N/Z) \to Z \times \mathbb{R}^{2n}$, which induces a Gysin map

$$d\iota_! : K^0(T(N/Z)) \to K^0(Z \times \mathbb{R}^{2n})$$

upon identifying $T^*(N/Z)$ with $T(N/Z)$. Let $j : Z \to Z \times \mathbb{R}^{2n}$ be the inclusion $j(z) = (z, 0)$. It induces the Bott isomorphism $j_! : K^0(Z) \cong K^0(Z \times \mathbb{R}^{2n})$. The topological index of the family D is, by definition,

$$\text{index}_t = j_!^{-1} \circ d\iota_! : K^0(T^*(N/Z)) \to K^0(Z)$$

The Atiyah–Singer (1971) index theorem for families of elliptic operators D asserts the equality of the analytic index and the topological index,

$$\text{index}(D) = \text{index}_t(\sigma(D)) \in K^0(Z)$$

Combined with the Grothendieck–Riemann–Roch theorem, one has the following exquisite formula in $H^\bullet(Z, \mathbb{Q})$:

$$\text{Ch}(\text{index}(D)) = \rho_* \pi_* \{\text{Todd}(T^*_{\mathbb{C}}(N/Z)) \cup \text{Ch}(\sigma(D))\}$$

where $\rho : T^*_{\mathbb{C}}(N/Z) \to N$ is the projection.

The map sending a complex vector bundle E over Z to its determinant line bundle $\det(E) = \Lambda^{\max} E$ induces a homomorphism, $\det : K^0(Z) \to \pi_0(\text{Pic}(Z))$, where $\pi_0(\text{Pic}(Z))$ denotes the isomorphism classes of complex line bundles over Z. Then

$$c_1(\det(\text{index}(D))) = \{\rho_* \pi_* \{\text{Todd}(T^*_{\mathbb{C}}(N/Z)) \cup \text{Ch}(\sigma(D))\}\}^{[2]}$$

where $^{[2]}$ denotes the degree-2 component, and the left-hand side denotes the first Chern class of the determinant line bundle of the index class. This formula is often used in the study of anomalies in physics.

K-Theory of C^*-Algebras

The Gelfand–Naimark theorem asserts that unital abelian C^*-algebras A can be identified with the space of continuous functions $C(X)$, where X is the compact Hausdorff space known as the spectrum of A, consisting of characters of A. Conversely, given a compact Hausdorff space X, the characters of $C(X)$ consist of the evaluation maps at points of X.

Let E be a vector bundle over X. Then there is a vector bundle F over X such that $E \oplus F \cong X \times \mathbb{C}^n$. Setting $A = C(X)$, $\mathcal{M} = C(X, E)$, $\mathcal{N} = C(X, F)$, we see that $\mathcal{M} \oplus \mathcal{N} \cong A^n$, showing that each vector bundle E over X determines a canonical finite projective module $\mathcal{M}$ over A. The converse is also true and is a result of Serre and Swan, cf. Blackadar (1986), which asserts that every finite projective module $\mathcal{M}$ over A is the space of all continuous sections of a vector bundle over X. So we have an equivalence of the category of vector bundles over X and the category of finite projective modules over A.

This motivates the following generalization of topological K-theory for a general unital C^*-algebra A. Let $\text{Proj}(A)$ denote the isomorphism classes of finite projective modules over A. It is a commutative semigroup under the operation of direct sum, which can be made into the commutative group $K_0(A)$ as follows: $K_0(A)$ is generated by pairs $([\mathcal{M}], [\mathcal{N}])$, together with the relation $([\mathcal{M}], [\mathcal{N}]) = ([\mathcal{M}'], [\mathcal{N}'])$ if $\mathcal{M} \oplus \mathcal{N}' \oplus \mathcal{G} \cong \mathcal{M}' \oplus \mathcal{N} \oplus \mathcal{G}$ for some $[\mathcal{G}] \in \text{Proj}$

(A). Also $K_1(A) = \pi_0(\mathrm{GL}(\infty, A))$ where $\mathrm{GL}(\infty, A)$ denotes the direct limit of $\mathrm{GL}(n, A)$ where $(\mathrm{GL}(n, A)$ embeds in $\mathrm{GL}(n+1, A)$ as $1 \oplus \mathrm{GL}(n, A)$. Then, defining $K_j(A) = \pi_{j-1}(\mathrm{GL}(\infty, A))$ for $j \geq 1$, together with generalized Bott periodicity which asserts that there is a canonical isomorphism $\pi_{j-1}(\mathrm{GL}(\infty, A)) \cong \pi_{j+1}(\mathrm{GL}\ (\infty, A))$, we see that $K_\bullet(A) = K_0(A) \oplus K_1(A)$ is a generalized periodic cohomology theory. If A is a C^*-algebra without unit, then consider $A^+ = A \oplus \mathbb{C}$, with product given by $(a, \lambda)(b, \mu) = (ab + a\mu + b\lambda, \lambda\mu)$ with unit $(0, 1)$. The projection $p : A^+ \to \mathbb{C}$ defined as $p(a, \lambda) = \lambda$ induces a map $p_! : K_\bullet(A^+) \to K_\bullet(\mathbb{C})$. In the nonunital case, $K_\bullet(A)$ is defined as $\ker(p_!)$. Observe that $K_1(A) = K_1(A^+)$, but this is often not the case with K_0. It is easy to see that when A has a unit, then the two definitions of K_0 agree. An important caveat in the case of noncommutative C^*-algebras is that the K-theory is often not a ring as there is no analog of the tensor product operation.

Some of the basic properties of K-theory are listed as follows. Details can be found in Blackadar (1986).

1. *Cup product* A continuous bilinear map of C^*-algebras, $A \times B \to C$, induces a cup product, $K_i(A) \otimes K_j(B) \to K_{i+j}(C)$.
   In particular, the continuous product $A \times A \to A$ induces a cup product homomorphism, $K_i(A) \otimes K_j(A) \to K_{i+j}(A)$.
2. *Induced homomorphism* If $f : A \to B$ is a homomorphism of C^*-algebras, then there is an induced homomorphism, $f_! : K_\bullet(A) \to K_\bullet(B)$.
3. *Homotopy* If $f : A \to B$ and $g : A \to B$ are homomorphisms of C^*-algebras that are homotopic, the induced homomorphisms on K-theory $f_* = g_*$ are equal.
4. *Excision* If I is a closed two-sided ideal in A, then there is a six-term exact sequence in K-theory,

$$\begin{array}{ccccc} K_0(I) & \longrightarrow & K_0(A) & \longrightarrow & K_0(A/I) \\ \uparrow & & & & \downarrow\Delta \\ K_1(A/I) & \longleftarrow & K_1(A) & \longleftarrow & K_1(I) \end{array}$$

5. *Morita invariance* The inclusion homomorphism of A into the top left of the diagonal in $M_n(A)$ induces an isomorphism in K-theory, $K_\bullet(A) \cong K_\bullet(M_n(A))$.
6. *Continuity* Let $A = \lim_{n \to \infty} A_n$ be a C^*-direct limit. Then, $K_\bullet(A) = \lim_{n \to \infty} K_\bullet(A_n)$.
7. *Stability* Let $\mathcal{K}$ be a C^*-algebra of all compact operators on an infinite-dimensional complex Hilbert space. Then since $\mathcal{K} = \lim_{n \to \infty} M_n(\mathbb{C})$ is a C^*-direct limit, we see that $K_\bullet(A \otimes \mathcal{K}) = \lim_{n \to \infty} K_\bullet(A \otimes M_n(\mathbb{C})) = K_\bullet(A)$.
8. *Bott periodicity* The continuous product $A \times \mathbb{C} \to A$ induces the cup product $K_i(A) \otimes K_j(\mathbb{C}) \to K_{i+j}(A)$. The computation by Bott asserts that there is a canonical element $b \in K_2(\mathbb{C})$ that gives an isomorphism $K_2(\mathbb{C}) \cong \mathbb{Z}$, and Bott periodicity asserts that the cup product with b gives rise to an isomorphism $K_i(A) \cong K_{i+2j}(A)$.

We mention in passing that Connes has defined a Chern character homomorphism, $\mathrm{Ch} : K_\bullet(A) \to HE_\bullet(A)$, mapping into the entire cyclic homology of A, having similar properties as the ordinary Chern character. Due to space constraints, it will not be defined here.

A C^*-Algebra Generalization of the Atiyah–Singer Index Theorem and the Baum–Connes Conjecture

We content ourselves here with a rudimentary account of the C^*-algebra generalization of the Atiyah–Singer index theorem and the Baum–Connes conjecture, and its relevance to the quantum Hall effect and strict deformation quantization. Let A be a C^*-algebra.

Let $\mathcal{H}_A = A \otimes \mathcal{H}$, which is the analog of a Hilbert space. Let $\mathcal{F}_A$ be the space of all A-Fredholm operators on $\mathcal{H}_A$. Recall that an operator T is said to be A-Fredholm if both the kernel and cokernel of $T + K$ are closed and finitely generated projective modules, where K is an A-compact operator. The space of A-compact operators is by definition the closure of the A-finite rank operators. The index of T is

$$\mathrm{index}(T) = [\ker(T + K)] - [\mathrm{coker}(T + K)] \in K_0(A)$$

The index map turns out to be well defined and independent of the choice of A-compact perturbation K. It is continuous, so it induces a map on the connected components of $\mathcal{F}_A$, which turns out to be an isomorphism, by a theorem of Mingo (cf. Rosenberg (1983, 1989)).

Now let M be a smooth compact manifold. An A-vector bundle over M is a locally trivial Banach vector bundle E over M whose fibers have the structure of finitely generated left A-modules, with morphisms respecting the A-module structure. The isomorphism classes of A-vector bundles over M form a commutative semigroup under direct sums, and the associated commutative group is easily identified with $K_0(C(M) \otimes A)$. Let $D : C^\infty(M, E) \to C^\infty(M, F)$ be an elliptic A-operator acting between smooth sections of A-vector bundles E, F over M. It

turns out that by elliptic regularity, such an operator is A-Fredholm, and has an analytic index,

$$\text{index}(D) \in K_0(A)$$

Associated to each such operator is a symbol

$$\sigma(D) : \pi^*(E) \to \pi^*(F)$$

where $\pi : T^*M \to M$ is the projection. Ellipticity is the condition that $\sigma(D)$ is an isomorphism outside the zero section, so that the triple $(\pi^*(E), \pi^*(F), \sigma(D))$ determines an element in $K_0(C_0(T^*M) \otimes A)$ denoted by $\sigma(D)$. It turns out that the analytic index of D depends only on the class $\sigma(D) \in K_0(C_0(T^*M) \otimes A)$. Therefore, the analytic index can be viewed as a homomorphism,

$$\text{index} : K_0(C_0(T^*M) \otimes A) \to K_0(A)$$

Consider an embedding $\iota : M \hookrightarrow \mathbb{R}^n$, which induces an embedding $d\iota : TM \to \mathbb{R}^{2n}$. The associated Gysin map is $d\iota_! : K_0(C_0(T^*M) \otimes A) \to K_0(C_0(\mathbb{R}^{2n}) \otimes A)$. Let $j : \{0\} \to \mathbb{R}^{2n}$ denote inclusion of the origin in $\mathbb{R}^{2n}$. It induces a Gysin map $j_! : K_0(A) \to K_0(C_0(\mathbb{R}^{2n}) \otimes A)$ which is the Bott periodicity isomorphism. Then the topological index is the homomorphism

$$\text{index}_t = j_!^{-1} \circ d\iota_! : K_0(C_0(T^*M) \otimes A) \to K_0(A)$$

The C^*-generalization of the Atiyah–Singer index theorem due to Mishchenko–Formenko, cf. Kasparov (1988), asserts the equality of the analytic index and the topological index,

$$\text{index}(D) = \text{index}_t(\sigma(D)) \in K_0(A)$$

Now let M be a compact even-dimensional $\text{spin}^{\mathbb{C}}$ manifold. Then there is a $\text{spin}^{\mathbb{C}}$ Dirac operator $D : C^\infty(M, S^+) \to C^\infty(M, S^-)$, where $S^\pm$ is the bundle of half-spinors on $T^*M \otimes L$, where L is a line bundle over M with the property that the first Chern class of L modulo 2, $c_1(L) \bmod 2$ is equal to the second Stieffel–Whitney class of M, $w_2(M)$. Let Γ be a torsion-free discrete group, and $B\Gamma$ be its classifying space. It is a paracompact space with the property that it is the quotient of Γ acting freely on a contractible space $E\Gamma$. Let $C_r^*(\Gamma)$ denote the reduced group C^*-algebra, and consider the canonical flat $C_r^*(\Gamma)$ bundle $\mathcal{V}$ over $B\Gamma$ defined as follows:

$$\mathcal{V} = \{E\Gamma \times C_r^*(\Gamma)\}/\Gamma$$

where Γ acts on the left on $C_r^*(\Gamma)$ and on the right on $E\Gamma$. Let $f : M \to B\Gamma$ be a continuous map. Then $f^*\mathcal{V}$ is a flat $C_r^*(\Gamma)$-bundle over M. Upon choosing a flat connection on $f^*\mathcal{V}$, we can couple the $\text{spin}^{\mathbb{C}}$ Dirac operator $D_{\mathcal{V}}$ to act on sections of $S^\pm \otimes f^*\mathcal{V}$. The ellipticity of $D_{\mathcal{V}}$ ensures that it is a $C_r^*(\Gamma)$-Fredholm operator, so it has an analytic index, $\text{index}(D_{\mathcal{V}}) \in K_0(C_r^*(\Gamma))$ by the earlier discussion, which is also equal to the topological index $\text{index}_t(\sigma(D_{\mathcal{V}})) \in K_0(C_r^*(\Gamma))$.

By Baum, Connes, and Douglas, the K-homology of $B\Gamma$, $K_0(B\Gamma)$, is generated by the triples (M, E, f) as described above, modulo relations that we will not present here because of space constraints. The assembly map

$$\mu : K_0(B\Gamma) \to K_0(C_r^*(\Gamma))$$

is a homomorphism given by $\mu([(M, E, f)]) = \text{index}(D_{\mathcal{V}})$. The Baum–Connes conjecture asserts that μ is an isomorphism. There are variants of this conjecture when Γ has torsion. The Baum–Connes conjecture has been verified when Γ is an amenable group or, for instance, a word hyperbolic group. There are also variants of this conjecture for certain foliations and groupoids, and is an extremely active area of research. The injectivity of the assembly map is related to the Novikov conjecture on the homotopy invariance of the higher signatures (Kasparov 1988), and the obstructions to the existence of Riemannian metrics of positive scalar curvature on compact spin manifolds (Rosenberg 1983, 1989). A variant of the Baum–Connes conjecture, where the reduced group C^*-algebra is replaced by the twisted reduced group C^*-algebra, is used in the analysis of the noncommutative geometry approach to the integer and fractional quantum Hall effect, and also the gaps in the spectrum of magnetic Schrödinger operators (Bellissard *et al.* 1994, Marcolli and Mathai 2001).

Twisted *K*-theory and the Chern Character

We begin by reviewing some results due to Dixmier and Douady (1963). Let M be a smooth manifold, let $\mathcal{H}$ denote an infinite-dimensional, separable, Hilbert space and let $\mathcal{K}$ be the C^*-algebra of compact operators on $\mathcal{H}$. Let $\text{U}(\mathcal{H})$ denote the group of unitary operators on $\mathcal{H}$ endowed with the strong operator topology and let $\text{PU}(\mathcal{H}) = \text{U}(\mathcal{H})/\text{U}(1)$ be the projective unitary group with the quotient space topology, where $\text{U}(1)$ consists of scalar multiples of the identity operator on $\mathcal{H}$ of norm equal to 1. Since $\text{U}(\mathcal{H})$ is contractible in the operator norm topology, it follows that $\text{PU}(\mathcal{H}) = B\text{U}(1)$ is an Eilenberg–MacLane space $K(\mathbb{Z}, 2)$. Therefore, $B\text{PU}(\mathcal{H})$ is an Eilenberg–MacLane space $K(\mathbb{Z}, 3)$. That is, principal $\text{PU}(\mathcal{H})$ bundles P over X are classified up to isomorphism by

the Dixmier–Douady class $DD(P)$ in $H^3(X,\mathbb{Z})$ and conversely.

For $g \in \mathrm{U}(\mathcal{H})$, let $\mathrm{Ad}(g)$ denote the automorphism $T \to gTg^{-1}$ of $\mathcal{K}$. As is well known, Ad is a continuous homomorphism of $\mathrm{U}(\mathcal{H})$, given the strong operator topology, onto $\mathrm{Aut}(\mathcal{K})$ with kernel the circle of scalar multiples of the identity where $\mathrm{Aut}(\mathcal{K})$ is given the point-norm topology. Under this homomorphism we may identify $\mathrm{PU}(\mathcal{H})$ with $\mathrm{Aut}(\mathcal{K})$. Define an Azumaya bundle to be a locally trivial bundle $\mathcal{E}$ over X with fiber $\mathcal{K}$ and structure group $\mathrm{Aut}(\mathcal{K})$. They are of the form $\mathcal{K}_P = \{P \times \mathcal{K}\}/\mathrm{PU}(\mathcal{H})$ and isomorphism classes of Azumaya bundles are also parametrized by their Dixmier–Douady class $\mathrm{DD}(P)$ in $H^3(X,\mathbb{Z})$ and conversely.

Since $\mathcal{K} \otimes \mathcal{K} \cong \mathcal{K}$, the isomorphism classes of locally trivial bundles over X with fiber $\mathcal{K}$ and structure group $\mathrm{Aut}(\mathcal{K})$ form a group under the tensor product, where the inverse of such a bundle is the conjugate bundle. This group is known as the infinite Brauer group and is denoted by $\mathrm{Br}^\infty(X)$. So, a restatement of the Dixmier–Douady theorem is that $\mathrm{Br}^\infty(X) \cong H^3(X,\mathbb{Z})$. $H^3(X,\mathbb{Z})$ can also be described in terms of bundle gerbes (Murray 1996).

The twisted K-theory, $K^\bullet(X,P)$, is defined as the K-theory of the C^*-algebra of continuous sections of the Azumaya bundle $\mathcal{K}_P, K_\bullet(C(X,\mathcal{K}_P))$. It was studied in the torsion case by Donovan and Karoubi, where one can replace the compact operators $\mathcal{K}$ by finite-dimensional matrices, and was studied in the general case by Rosenberg (1983, 1989). Let $\mathcal{F}$ be the space of all Fredholm operators endowed with the norm topology. Then, one can form the bundle of Fredholm operators $\mathcal{F}_P = \{P \times \mathcal{F}\}/\mathrm{PU}(\mathcal{H})$, where $\mathrm{PU}(\mathcal{H})$ acts on $\mathcal{F}$ via the adjoint action. Consider the fibration $\mathcal{K}_P \to \mathcal{F}_P \to \mathrm{GL}(\mathcal{C}_P)$, where $\mathcal{C}_P = \{P \times \mathcal{C}\}/\mathrm{PU}(\mathcal{H})$ and $\mathcal{C} = \mathcal{B}(\mathcal{H})/\mathcal{K}$ is the Calkin algebra. Since $\pi_0(C(X,\mathcal{K}_P)) = \{0\}$, we see that $\pi_0(C(X,\mathcal{F}_P)) = \pi_0(C(X,\mathrm{GL}(\mathcal{C}_P)))$. Consider the short exact sequence of C^*-algebras,

$$0 \to C(X,\mathcal{K}_P) \to C(X,\mathcal{B}_P) \to C(X,\mathcal{C}_P) \to 0$$

where $\mathcal{B}_P = \{P \times \mathcal{B}(\mathcal{H})\}/\mathrm{PU}(\mathcal{H})$ and where $\mathrm{PU}(\mathcal{H})$ acts on $\mathcal{B}(\mathcal{H})$ via the adjoint action. It gives rise to a six-term exact sequence

$$\begin{array}{ccccc} K_0(C(X,\mathcal{K}_P)) & \longrightarrow & K_0(C(X,\mathcal{B}_P)) & \longrightarrow & K_0(C(X,\mathcal{C}_P)) \\ \text{index}\uparrow & & & & \downarrow \\ K_1(C(X,\mathcal{C}_P)) & \longleftarrow & K_1(C(X,\mathcal{B}_P)) & \longleftarrow & K_1(C(X,\mathcal{K}_P)) \end{array}$$

By definition, $K_1(C(X,\mathcal{C}_P)) \cong \pi_0(C(X,\mathrm{GL}(\infty,\mathcal{C}_P)))$ and a standard argument shows that this is also equal to $\pi_0(C(X,\mathrm{GL}(\mathcal{C}_P)))$. By Kuiper's theorem, it is not difficult to see that $K_\bullet(C(X,\mathcal{B}_P)) = \{0\}$. Therefore,

$$\text{index}: \pi_0(C(X,\mathcal{F}_P)) \to K^0(X,P)$$

is an isomorphism. Let X_1 be a closed subset of X, and I_{X_1} be the closed ideal of sections of $\mathcal{K}_P$ that vanish on X_1. Then $K^\bullet(X,X_1,P)$ is by definition $K_\bullet(I_{X_1})$. A geometric description of twisted K-theory in terms of modules for bundle gerbes is described in Bouwknegt *et al.* (2002).

Some of the basic properties of twisted K-theory are listed as follows. Many of these properties follow from the corresponding properties for the K-theory of C^*-algebras. See Atiyah and Segal and Bouwknegt *et al.* (2002).

1. *Normalization* If P is trivial, then $K^\bullet(M,P) = K^\bullet(M)$.
2. *Module property* $K^\bullet(M,P)$ is a module over $K^0(M)$.
3. *Pullback* If $f: N \to M$ is a continuous map, and P a principal $\mathrm{PU}(\mathcal{H})$ bundle over M, then there is a pullback homomorphism $f: K^\bullet(M,P) \to K^\bullet(N,f(P))$.
4. *Push-forward* Let $f: N \to M$ be a smooth proper map between compact manifolds which is K-oriented, that is, $TN \oplus f^*TM$ is a spin$^{\mathbb{C}}$ vector bundle over N. Let P be a principal $\mathrm{PU}(\mathcal{H})$ bundle over M. Then there is a pushforward homomorphism, also called a Gysin map, $f: K^\bullet(N,f^!(P)) \to K^{\bullet+d}(M,P)$, where $d = \dim M - \dim N$.
5. *Homotopy* If $f: N \to M$ and $g: N \to M$ are homotopic maps, then the pullback maps $f^! = g^!$ are equal. If in addition, f and g are K-oriented, then the pushforward maps $f_! = g_!$ are equal.
6. *Excision* Let M_1 be a closed subset of M and U be an open subset of M such that U is contained in the interior of M_1. Then the inclusion of pairs $(M\backslash U, M_1\backslash U) \hookrightarrow (M, M_1)$ induces an isomorphism in K-theory, $K^\bullet(M,M_1,P) \cong K^\bullet(M\backslash U, M_1\backslash U, P|_{M\backslash U})$.
7. *Exactness* Let M_1 be a closed subset of M and $\iota: M_1 \to M$ be the inclusion. Let P be a principal $\mathrm{PU}(\mathcal{H})$ bundle over M. Then the short exact sequence

$$0 \to I_{M_1} \to C(M,\mathcal{K}_P) \to C\left(M_1, \mathcal{K}_{P|_{M_1}}\right) \to 0$$

gives rise to the six-term exact sequence in K-theory,

$$\begin{array}{ccccc} K^0(M,M_1,P) & \longrightarrow & K^0(M,P) & \longrightarrow & K^0(M_1,\iota^!(P)) \\ \uparrow & & & & \downarrow\Delta \\ K^1(M_1,\iota^!(P)) & \longleftarrow & K^1(M,P) & \longleftarrow & K^1(M,M_1,P) \end{array}$$

8. *Cup product* Let P be a principal $\mathrm{PU}(\mathcal{H})$ bundle over M and Q be a principal $\mathrm{PU}(\mathcal{H})$ bundle over N. An identification $\mathcal{H} \otimes \mathcal{H} \cong \mathcal{H}$ gives rise to a principal $\mathrm{PU}(\mathcal{H})$ bundle $P \otimes Q$ over $M \times N$ whose Dixmier–Douady invariant is $DD(P \otimes Q) = p_1^*(DD(P)) + p_2^*(DD(Q))$, where p_j denote projections onto the jth factor, $j = 1, 2$. Then there is a canonical map given by external tensor product,

   $$K^i(M, P) \otimes K^j(N, Q) \to K^{i+j}(M \times N, P \otimes Q)$$

   called the cup product.
9. *Bott periodicity* Let P be a principal $\mathrm{PU}(\mathcal{H})$ bundle over M. Bott periodicity says that there is a canonical isomorphism

   $$K^\bullet(M, P) \cong K^{\bullet+n}(M \times \mathbb{R}^n, \pi(P))$$

   where $\pi : M \times \mathbb{R}^n \to M$ is the projection onto the first factor. Let $b \in K^n(\mathbb{R}^n)$ be the Bott element. Then the isomorphism above is given by $\pi^!(x) \cup b \in K^{\bullet+n}(M \times \mathbb{R}^n, \pi^!(P))$ for all $x \in K^\bullet(M, P)$.

There is a natural homomorphism of rings called the twisted Chern character, which depends both on a choice of P and a de Rham representative H of $DD(P)$,

$$\mathrm{Ch}_P : K^\bullet(M, P) \to H^\bullet(M, H)$$

Here $H^\bullet(M, H)$ denotes the twisted cohomology, which is by definition the cohomology of the complex $(\Omega^\bullet(M), d - H\wedge)$. The twisted Chern character is characterized by the following axioms:

1. *Naturality* If $f : N \to M$ is a smooth map, and if $x \in K^\bullet(M, P)$, then $\mathrm{Ch}_{f(P)}(f^!(x)) = f^*(\mathrm{Ch}_P(x))$.
2. *Additivity* If $x, y \in K^\bullet(M, P)$, then $\mathrm{Ch}_P(x \oplus y) = \mathrm{Ch}_P(x) + \mathrm{Ch}_P(y)$.
3. Ch_P respects the $K^0(M)$-module structure of $K^0(M, P)$.
4. *Normalization* If P is trivial, then Ch_P reduces to the ordinary Chern character Ch.

It turns out that the twisted Chern character induces an isomorphism of the rings $K^\bullet(M, P) \otimes \mathbb{Q}$ and $H^\bullet(M, H)$. The Chern–Weil representative of the twisted Chern character is derived in Bouwknegt *et al.* (2002).

Twisted *K*-Theory and Duality in Type II String Theories

Let E be an oriented S^1-bundle over M,

$$\begin{array}{ccc} S^1 & \longrightarrow & E \\ & & \pi\downarrow \\ & & M \end{array}$$

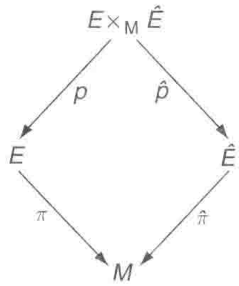
characterized by its first Chern class $c_1(E) \in H^2(M, \mathbb{Z})$, in the presence of (possibly nontrivial) H-flux $H \in H^3(E, \mathbb{Z})$. We will argue that the T-dual of E is again an oriented S^1-bundle over M, denoted by $\hat{E}$,

$$\begin{array}{ccc} \hat{S}^1 & \longrightarrow & \hat{E} \\ & & \hat{\pi}\downarrow \\ & & M \end{array}$$

supporting H-flux $\hat{H} \in H^3(\hat{E}, \mathbb{Z})$, such that

$$c_1(\hat{E}) = \pi_* H, \qquad c_1(E) = \hat{\pi}_* \hat{H}$$

where $\pi_* : H^k(E, \mathbb{Z}) \to H^{k-1}(M, \mathbb{Z})$ and, similarly, $\hat{\pi}_*$ denote the pushforward maps. Then we can form the following commutative diagram:



The correspondence space $E \times_M \hat{E}$ is a circle bundle over E with first Chern class $\pi^*(c_1(\hat{E}))$, and it is also a circle bundle over $\hat{E}$ with first Chern class $\hat{\pi}^*(c_1(E))$, by the commutativity of the diagram above. If $\hat{E} = E$ or if $\hat{E} = M \times S^1$, then the correspondence space $E \times_M \hat{E}$ is diffeomorphic to $E \times S^1$.

T-duality gives an isomorphism of the twisted K-theories of E and $\hat{E}$ as well as an isomorphism between the twisted cohomologies of E and $\hat{E}$, and can be expressed in the following commutative diagram:

$$\begin{array}{ccc} K^\bullet(E, P) & \xrightarrow{T} & K^{\bullet+1}(\hat{E}, \hat{P}) \\ \mathrm{Ch}_P\downarrow & & \downarrow\mathrm{Ch}_{\hat{P}} \\ H^\bullet(E, H) & \xrightarrow{T_*} & H^{\bullet+1}(\hat{E}, \hat{H}) \end{array}$$

where the horizontal arrows are isomorphisms. Here P is a principal $\mathrm{PU}(\mathcal{H})$ bundle over E such that $DD(P) = H$ and $\hat{P}$ is a principal $\mathrm{PU}(\mathcal{H})$ bundle over $\hat{E}$ such that $DD(\hat{P}) = H$. We refer to Bouwknegt *et al.* (2004) for details. The T-duality isomorphism above gives compelling evidence that a type II*A* string theory A on a circle bundle of radius R in the presence of a background H-flux, and a type II*B* string theory B on a "T-dual" circle bundle of radius

$1/R$ in the presence of a "T-dual" background H-flux, are equivalent in the sense that the string states of string theory A are in canonical one-to-one correspondence with the string states of string theory B.

We briefly mention two other applications of twisted K-theory. Consider the adjoint action of a compact connected simple Lie group G on itself, and the corresponding twisted G-equivariant K-theory, twisted by a multiple of the generator of $H^3(G, \mathbb{Z})$. The relevance of the equivariant case to conformal field theory was highlighted by the result of Freed, Hopkins and Teleman (see Freed (2002)) that it is graded isomorphic to the Verlinde algebra of G, with a shift given by the dual Coxeter number. Here the Verlinde algebra consists of equivalence classes of positive-energy representations of the loop group of G which was originally shown to be a ring in a rather nontrivial way. On the other hand, the ring structure of the twisted G-equivariant K-theory of G is just induced by the product on G, which makes this result all the more remarkable.

Fractional analytic index theory, developed in Mathai *et al.* is a generalization of Atiyah–Singer index theory, assigning a fractional-valued analytic index to each projective elliptic operator on a compact manifold, where the fraction need not be an integer. These projective elliptic operators act on projective vector bundles, where the usual compatibility condition on triple overlaps to give a global vector bundle, may fail by a scalar factor. These are the geometric objects in twisted K-theory, when the twist is torsion. In Mathai *et al.*, a fractional index theorem is proved, computing the fractional-valued analytic index of projective elliptic operators essentially in terms of topological data. The Dirac operator in the absence of a spin structure is also defined there for the first time resolving a long standing mystery, and its index is computed.

Some topics not covered in this brief account of K-theory include: KK-theory, cf. Blackadar (1986) and Kasparov (1988), which is natural setting for the Atiyah–Singer index theorem and its generalizations, as well as higher algebraic K-theory.

See also: C^*-Algebras and Their Classification; Characteristic Classes; Cohomology Theories; Equivariant Cohomology and the Cartan Model; Gerbes in Quantum Field Theory; Index Theorems; Intersection Theory; Mathai–Quillen Formalism; Spectral Sequences.

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Lagrangian Dispersion (Passive Scalar)

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Introduction

To describe transport by a random flow, one needs to apply the statistical methods to the motion of fluid particles, that is, to the Lagrangian dynamics. We first present the propagators describing evolving probability distributions of different configurations of fluid particles. We then use those propagators to describe decay and steady states of a passive scalar field transported by random flows.

Consider an evolution of a passive scalar tracer $\theta(\boldsymbol{r},t)$ in a random flow. The mean value of the scalar tracer at a given point is an average over values brought by different trajectories:

$$\langle\theta(\boldsymbol{r},s)\rangle = \int \mathcal{P}(\boldsymbol{r},s;\boldsymbol{R},0)\,\theta(\boldsymbol{R},0)\,\mathrm{d}\boldsymbol{R} \qquad [1]$$

Here, $\mathcal{P}(\boldsymbol{r},s;\boldsymbol{R},t)$ is the probability density function (PDF) to find the particle at time t at position $\boldsymbol{R}$ given its position $\boldsymbol{r}$ at time s. That PDF is called the propagator or the Green function. Multipoint correlation functions of the tracer

$$C_N(\underline{\boldsymbol{r}},s) \equiv \langle\theta(\boldsymbol{r}_1,s)\ldots\theta(\boldsymbol{r}_N,s)\rangle = \int \mathcal{P}_N(\underline{\boldsymbol{r}},s;\underline{\boldsymbol{R}},0)\,\theta(\boldsymbol{R}_1,0)\ldots\theta(\boldsymbol{R}_N,0)\,\mathrm{d}\underline{\boldsymbol{R}} \qquad [2]$$

are expressed via the multiparticle Green functions $\mathcal{P}_N$ which are the joint PDFs of the equal-time positions $\underline{\boldsymbol{R}}=(\boldsymbol{R}_1,\ldots,\boldsymbol{R}_N)$ of N fluid trajectories.

The trajectory of the fluid particle that passes at time s through the point $\boldsymbol{r}$ is described by the vector $\boldsymbol{R}(t;\boldsymbol{r},s)$ which satisfies $\boldsymbol{R}(t;\boldsymbol{r},t)=\boldsymbol{r}$ and the stochastic equation

$$\dot{\boldsymbol{R}} = \boldsymbol{v}(\boldsymbol{R},t) + \boldsymbol{u}(t) \qquad [3]$$

Here, $\boldsymbol{u}(t)$ describes the molecular Brownian motion with zero average and covariance $\langle u^i(t)u^j(t')\rangle = 2\kappa\delta^{ij}\delta(t-t')$. We also consider macroscopic velocity $\boldsymbol{v}$ as random with various statistical properties in space and time. There is a clear scale separation between macroscopic velocity $\boldsymbol{v}$ and molecular diffusion $\boldsymbol{u}$ that allows one to treat them separately.

Using [3], one can write the Green's function as an integral over paths that satisfy $\boldsymbol{q}(s)=\boldsymbol{r}$ and $\boldsymbol{q}(t)=\boldsymbol{R}$:

$$\mathcal{P}(\boldsymbol{r},s;\boldsymbol{R},t) = \left\langle \int \mathcal{D}p\mathcal{D}q \exp\left(-\int_s^t \imath\boldsymbol{p}(\tau)\cdot[\dot{\boldsymbol{q}}(\tau) - \boldsymbol{v}(\boldsymbol{q}(\tau),\tau) - \boldsymbol{u}(\tau)]\,\mathrm{d}\tau\right)\right\rangle_{v,u} \qquad [4]$$

$$= \left\langle \int \mathcal{D}p\mathcal{D}q \exp\left(-\int_s^t [\imath\boldsymbol{p}(\tau)\cdot(\dot{\boldsymbol{q}}(\tau) - \boldsymbol{v}(\boldsymbol{q}(\tau),\tau)) + \kappa p^2(\tau)]\,\mathrm{d}\tau\right)\right\rangle_{v} \qquad [5]$$

$$= \left\langle \int \mathcal{D}q \exp\left(-\frac{1}{4\kappa}\int_s^t [\dot{\boldsymbol{q}}(\tau) - \boldsymbol{v}(\boldsymbol{q}(\tau),\tau)]^2\,\mathrm{d}\tau\right)\right\rangle_{v} = \langle P(\boldsymbol{r},s;\boldsymbol{R},t|\boldsymbol{v})\rangle_v \qquad [6]$$

The integration over the auxiliary field $\boldsymbol{p}$ in [4] enforces the delta function of [3]. One passes from [4] to [5] by averaging over the Gaussian Brownian noise, and from [5] to [6] by calculating Gaussian integral over $\boldsymbol{p}$.

Generally, exact calculations are only possible for Gaussian random processes short-correlated in time-like in [5]. The simplest case is the Brownian motion when the advection is absent. One then obtains from [6] the Gaussian PDF of the displacement:

$$\mathcal{P}(\boldsymbol{R},t) = (4\pi\kappa t)^{-d/2}\mathrm{e}^{-R^2/(4\kappa t)} \qquad [7]$$

which satisfies the heat equation $(\partial_t - \kappa\nabla^2)\,\mathcal{P}(\boldsymbol{r},t)=0$. The short-correlated case is far from being an exotic exception but rather presents a long-time limit of an integral of any finite-correlated random function. Indeed, such an integral can be presented as a sum of many independent equally distributed random numbers,

the statistics of such sums is a subject of the central limit theorem. One can move beyond the central limit theorem considering the correlation time finite (yet small comparing to the time of evolution). Such generalization is the subject of the large deviation theory. Consider some quantity X which is an integral of some random function over time t much larger than the correlation time τ. At $t \gg \tau$, X behaves as a sum of many independent identically distributed random numbers y_i: $X = \sum_1^N y_i$ with $N \propto t/\tau$. The generating function $\langle e^{zX} \rangle$ of the moments of X is the product, $\langle e^{zX} \rangle = e^{NS(z)}$, where we have denoted $\langle e^{zy} \rangle \equiv e^{S(z)}$ (assuming that the generating function $\langle e^{zy} \rangle$ exists for all complex z). The PDF $\mathcal{P}(X)$ is given by the inverse Laplace transform $(2\pi i)^{-1} \int e^{-zX+NS(z)}\,dz$ with the integral over any axis parallel to the imaginary one. For $X \propto N$, the integral is dominated by the saddle point z_0 such that $S'(z_0) = X/N$ and

$$\mathcal{P}(X) \propto e^{-NH(X/N - \langle y \rangle)} \qquad [8]$$

Here $H = -S(z_0) + z_0 S'(z_0)$ is the function of the variable $X/N - \langle y \rangle$; it is called entropy function as it appears also in the thermodynamic limit in statistical physics. A few important properties of H (also called rate or Cramér function) may be established independently of the distribution $\mathcal{P}(y)$. It is a convex function which takes its minimum at zero, that is, for X equal to the mean value $\langle X \rangle = NS'(0)$. The minimal value of H vanishes since $S(0) = 0$. The entropy is quadratic around its minimum with $H''(0) = \Delta^{-1}$, where $\Delta = S''(0)$ is the variance of y. We thus see that the mean value $\langle X \rangle = N\langle y \rangle$ grows linearly with N. The fluctuations $X - \langle X \rangle$ on the scale $\mathcal{O}(N^{1/2})$ are governed by the central limit theorem that states that $(X - \langle X \rangle)/N^{1/2}$ becomes for large N a Gaussian random variable with variance $\langle y^2 \rangle - \langle y \rangle^2 \equiv \Delta$ as in [7]. Finally, its fluctuations on the larger scale $\mathcal{O}(N)$ are governed by the large deviation form [8]. The possible non-Gaussianity of the y's leads to a nonquadratic behavior of H for (large) deviations from the mean, starting from $X - \langle X \rangle / N \simeq \Delta / S'''(0)$. Note that if y is Gaussian, then X is Gaussian too for any t, but the universal formula [8] with $H = (X - N\langle y \rangle)^2 / 2N\Delta$ is valid only for $t \gg \tau$.

Single-Particle Diffusion

For the pure advection without noise, the displacement of the single Lagrangian trajectory is $\boldsymbol{R}(t) - \boldsymbol{R}(0) = \int_0^t \boldsymbol{V}(s)\,ds$, with $\boldsymbol{V}(t) = \boldsymbol{v}(\boldsymbol{R}(t), t)$ being the Lagrangian velocity. One can show that $\boldsymbol{V}(t)$ is statistically stationary in the frame of reference with no mean flow and under statistical homogeneity and stationarity of the incompressible Eulerian velocities. For $\kappa = 0$, the mean square displacement satisfies the equation

$$\frac{d}{dt}\langle [\boldsymbol{R}(t) - \boldsymbol{R}(0)]^2 \rangle = 2\int_0^t \langle \boldsymbol{V}(0) \cdot \boldsymbol{V}(s) \rangle\,ds \qquad [9]$$

The behavior of the displacement is crucially dependent on the Lagrangian correlation time τ of $\boldsymbol{V}(t)$ defined by

$$\int_0^\infty \langle \boldsymbol{V}(0) \cdot \boldsymbol{V}(s) \rangle\,ds = \langle \boldsymbol{v}^2 \rangle \tau \qquad [10]$$

No general relation between the Eulerian and the Lagrangian correlation times has been established, except for the case of short-correlated velocities. For times $t \ll \tau$, the two-point function in [9] is approximately equal to $\langle \boldsymbol{V}(0)^2 \rangle = \langle \boldsymbol{v}^2 \rangle$. The fluid particle transport is then ballistic with $\langle [\boldsymbol{R}(t) - \boldsymbol{R}(0)]^2 \rangle \simeq \langle \boldsymbol{v}^2 \rangle t^2$ and the PDF $\mathcal{P}(\boldsymbol{R}, t)$ is determined by the whole single-time velocity PDF. When the correlation time of $\boldsymbol{V}(t)$ is finite (a generic situation in a turbulent flow where τ is of order of a large-scale turnover time), an effective diffusive regime is expected to arise for $t \gg \tau$ with $\langle (\boldsymbol{R}(t) - \boldsymbol{R}(0))^2 \rangle \simeq 2\langle \boldsymbol{v}^2 \rangle \tau t$. Indeed, the particle displacements over time segments much larger than τ are almost independent. At long times, the displacement $\delta\boldsymbol{R}(t)$ behaves then as a sum of many independent variables and falls into the class of stationary processes treated in the previous section. In other words, $\delta\boldsymbol{R}(t)$ for $t \gg \tau$ becomes a Brownian motion in d dimensions, normally distributed with $\langle \delta R^i(t) \delta R^j(t) \rangle \simeq D_e^{ij} t$, where the so-called eddy diffusivity tensor is as follows:

$$D_e^{ij} = \frac{1}{2}\int_0^\infty \langle V_i(0)V_j(s) + V_j(0)V_i(s) \rangle\,ds \qquad [11]$$

The symmetric second-order tensor D_e^{ij} is the only characteristics of the velocity which matters in this limit of $t \gg \tau$. The trace of the tensor is equal to $\langle \boldsymbol{v}^2 \rangle \tau$, that is, equal to the large-time value of the integral in [9], while its tensorial properties reflect the rotational symmetries of the advecting velocity field. If the latter is isotropic, the tensor reduces to a diagonal form characterized by a single scalar value D_e. The main problem of turbulent diffusion is to obtain the effective diffusivity tensor given the velocity field $\boldsymbol{v}$ and the value of the molecular diffusivity κ.

Two-Particle Dispersion in Smooth Flows

Even when velocity $\boldsymbol{v}(\boldsymbol{R}, t)$ is a smooth function of the coordinates, Lagrangian dynamics can be quite

complicated. Indeed, d ordinary differential equations $\dot{R} = v(R, t)$ generally produce chaotic dynamics (for $d \geq 3$ already for steady flows and for $d = 2$ for time-dependent flows). The tools for the description of what is called chaotic advection are similar to those of the theory of dynamical chaos. The description consistently exploits two simple ideas: to single out the variables that can be represented by the sum of a large number of independent random quantities and to separate variables that fluctuate on different timescales.

The distance, $R_{12} = R_1 - R_2$, between two fluid particles with trajectories $R_i(t) = R(t; r_i)$ passing at $t = 0$ through points r_i satisfies the equation

$$\dot{R}_{12} = v(R_1, t) - v(R_2, t) \qquad [12]$$

If the velocity field can be considered smooth on the scale R_{12}, then one expands $v(R_1, t) - v(R_2, t) = \sigma(t, R_1)R_{12}$, introducing the strain matrix σ which can be treated as independent of R_{12}. The distance thus satisfies locally a linear system of ordinary differential equations (we omit subscripts replacing R_{12} by R)

$$\dot{R}(t) = \sigma(t)R(t) \qquad [13]$$

This equation, with the strain treated as given and $R(0) = r$, may be explicitly solved for arbitrary $\sigma(t)$ only in the 1D case

$$\ln[R(t)/r] = \ln W(t) = \int_0^t \sigma(s)\,ds \equiv X \qquad [14]$$

When t is much larger than the correlation time τ of the strain, the variable X is a sum of N independent equally distributed random numbers with $N = t/\tau$ and one can apply [8]. In the multidimensional case, to use the large deviation theory, one introduces the evolution matrix W such that $R(t) = W(t)R(0)$. The modulus R is expressed via the positive symmetric matrix $W^{T}W$. In almost every realization of the strain, the matrix $t^{-1}\ln W^{T}W$ stabilizes at $t \to \infty$, that is, its eigenvectors tend to d-fixed orthonormal eigenvectors f_i. To understand that intuitively, consider some fluid volume, say a sphere, which evolves into an elongated ellipsoid at later times. As time increases, the ellipsoid is more and more elongated and it is less and less likely that the hierarchy of the ellipsoid axes will change. The limiting eigenvalues

$$\lambda_i = \lim_{t\to\infty} t^{-1} \ln|Wf_i| \qquad [15]$$

are called Lyapunov exponents. The major property of the Lyapunov exponents is that they are realization independent if the flow is ergodic (i.e., spatial and temporal averages coincide). The relation [15] states that two fluid particles separated initially by r pointing into the direction f_i will separate (or converge) asymptotically as $\exp(\lambda_i t)$. The incompressibility constraints $\det(W) = 1$ and $\sum \lambda_i = 0$ imply that a positive Lyapunov exponent will exist whenever at least one of the exponents is nonzero. Consider indeed

$$E(n) = \lim_{t\to\infty} t^{-1} \ln\langle[R(t)/r]^n\rangle \qquad [16]$$

whose derivative at the origin gives the largest Lyapunov exponent λ_1. The function $E(n)$ obviously vanishes at the origin. Furthermore, $E(-d) = 0$, that is, incompressibility and isotropy make that $\langle R^{-d}\rangle$ is time independent as $t \to \infty$. Apart from $n = 0$, $-d$, the convex function $E(n)$ cannot have other zeroes if it does not vanish identically. It follows that dE/dn at $n = 0$, and thus λ_1, is positive. A simple way to appreciate intuitively the existence of a positive Lyapunov exponent is to consider the saddle-point 2D flow $v_x = \lambda x, v_y = -\lambda y$ with the axes randomly rotating after time interval T. A vector initially at the angle ϕ with the x-axis will be stretched after time T if $\cos\phi \geq [1 + \exp(2\lambda T)]^{-1/2}$, that is, the measure of the stretching directions is larger than $1/2$.

A major consequence of the existence of a positive Lyapunov exponent for any random incompressible flow is the exponential growth of the interparticle distance $R(t)$. In a smooth flow, it is also possible to analyze the statistics of the set of vectors $R(t)$ and to establish a multidimensional analog of [8]. The idea is to reduce the d-dimensional problem to a set of d scalar problems for slowly fluctuating stretching variables excluding the fast fluctuating angular degrees of freedom. Consider the matrix $I(t) = W(t)W^{T}(t)$, representing the tensor of inertia of a fluid element such as the above-mentioned ellipsoid. The matrix is obtained by averaging $R^i(t)R^j(t)d/\ell^2$ over the initial vectors of length ℓ and $I(0) = 1$. Introducing the variables that describe stretching as the lengths of the ellipsoid axis $e^{2\rho_1}, \ldots, e^{2\rho_d}$, one can deduce similarly to [8] the asymptotic PDF:

$$\begin{aligned}\mathcal{P}(\rho_1, \ldots, \rho_d; t) &\\ \propto \exp[-tH(\rho_1/t - \lambda_1, \ldots, \rho_{d-1}/t - \lambda_{d-1})]&\\ \times\, \theta(\rho_1 - \rho_2)\ldots\theta(\rho_{d-1} - \rho_d)&\\ \times\, \delta(\rho_1 + \cdots + \rho_d)&\end{aligned} \qquad [17]$$

The entropy function H depends on the statistics of σ. In the δ-correlated case, H is everywhere quadratic:

$$H(x) \propto d^{-1}\sum_{i=1}^{d} x_i^2, \qquad \lambda_i \propto d(d - 2i + 1) \qquad [18]$$

Two-Particle Dispersion in Nonsmooth Flows

To consider dispersion in the inertial interval of turbulence, one should assume $\delta v(r,t)| \propto r^{\alpha}$, where generally $\alpha < 1$. Rewriting then eqn [12] for the distance between two particles as $\dot{R} = \delta v(R,t)$, we infer that $dR^2/dt = 2R \cdot \delta v(R,t) \propto R^{1+\alpha}$. It suggests

$$R(t)^{1-\alpha} - R(0)^{1-\alpha} \propto t \qquad [19]$$

For large t, $R(t) \propto t^{1/(1-\alpha)}$, with the dependence of the initial separation quickly forgotten. Of course, for the random process $R(t)$, relation [19] is of the mean-field type and should pertain (if true) to the large-time behavior of the averages ($\langle R(t)^p \rangle \propto t^{p/(1-\alpha)}$, for $p > 0$) implying their super-diffusive growth, faster than the diffusive one $\propto t^{p/2}$. The power-law scaling may be amplified to the scaling behavior of the PDF of the interparticle distance, $\mathcal{P}(R,t) = \lambda\mathcal{P}(\lambda R, \lambda^{1-\alpha}t)$. The power-law growth of the second moment, $\langle R(t)^2 \rangle \propto t^3$, is the celebrated Richardson dispersion relation, which was the first quantitative phenomenological prediction in developed turbulence. It seems to be confirmed by experimental data and the numerical simulations. It is important to remark that, even assuming the validity of the Richardson relation, it is impossible to establish general large-time properties of the PDF $\mathcal{P}(R;t)$ such as those for the single-particle PDF of the distance between two particles. This is because the correlation time of the Lagrangian velocity difference, $R/\delta v(R) \propto \langle R^2 \rangle^{1/3} \propto t$, is comparable with the total time of the process.

It is instructive to contrast the exponential growth [16] of the distance between the trajectories with the power-law growth [19]. In a smooth flow, the closer two trajectories are initially, the more time is needed to effectively separate them. In a nonsmooth turbulent flow, the trajectories separate in a finite time independent of their initial distance $R(0)$, provided that the latter is also in the inertial range. This explosive separation of trajectories results in a breakdown of the deterministic Lagrangian flow since the trajectories cannot be labeled by the initial conditions. That agrees with the fundamental theorem stating that the ordinary differential equation $\dot{R} = v(R,t)$ does not have unique solution if $v(r,t)$ is non-Lipschitz. As shown by the example of the equation $\dot{x} = |x|^{\alpha}$ with two solutions $x = [(1-\alpha)t]^{1/(1-\alpha)}$ and $x = 0$ both starting at zero, one should expect multiple Lagrangian trajectories starting or ending at the same point for velocity fields with $\alpha < 1$. Even though the deterministic Lagrangian description breaks down, the statistical description is still possible and one can make sense of propagators like $P(r,s;R,t|v)$. They are expected to be weak solutions of the equation $[\partial_t - \nabla \cdot v(R,t)]P(r,s;R,t|v) = 0$ in the nonsmooth case. According to this assumption, the Lagrangian trajectories behave stochastically already in a given velocity field and for negligible molecular diffusivity – and not only due to a random noise or to random fluctuations of the velocities.

The general conjecture about the existence and diffuse nature of propagators is known to be true for the Gaussian ensemble of velocities decorrelated in time (Kraichnan 1968):

$$\langle v_i(r,t)v_j(r',t') \rangle = 2\delta(t-t')D_{ij}(r-r') \qquad [20]$$

Here the Lagrangian velocity $v(R,t)$ has the same white noise temporal statistics as the Eulerian velocity $v(r,t)$ for fixed r and the displacement along a Lagrangian trajectory $R(t) - R(0)$ is a Brownian motion for all times. To model nonsmooth velocity field of turbulence, we choose $D^{ij}(r) = D_0\delta^{ij} - (1/2)d^{ij}(r)$ and

$$d^{ij}(r) = D_1[(d-1+\xi)\delta^{ij}r^{\xi} - \xi r^i r^j r^{\xi-2}] \qquad [21]$$

Here D_0 gives the eddy diffusivity of a single fluid particle (discussed earlier), whereas $d_{ij}(r)$ describes the statistics of the velocity differences. For $0 < \xi < 2$, the Kraichnan ensemble is supported on the velocities that are Hölder continuous in space with a fixed exponent α arbitrarily close to $\xi/2$. It mimics this way the main property of turbulent velocities. The rough (distributional) behavior of Kraichnan velocities in time, although not very physical, is not expected to modify essentially the qualitative properties of propagators (it is the spatial regularity, not the temporal one, of a vector field that is crucial for the uniqueness of its trajectories).

In exactly the same way as one derives [6] and [7] from [4], one gets $\mathcal{P}(R,t) = |\hat{\beta}|^{1/2}(4\pi t)^{-d/2}e^{-\beta_{ij}R_iR_j/4t}$, where $(\hat{\beta}^{-1})_{ij} = D_{ij}(0) + \kappa\delta_{ij}$. In much the same way one can examine the two-particle PDF. The PDF $\mathcal{P}_2(r,s;R,t)$ of the distance R between two particles satisfies the equation

$$(\partial_t - M_2)\mathcal{P}_2(r,s;R,t) = \delta(t-s)\delta(r-R) \qquad [22]$$

where $M_2 = -D_1(d-1)r^{1-d}\partial_r r^{d-1+\xi}\partial_r$ and [22] can be readily solved:

$$\lim_{r\to 0}\mathcal{P}_2(r,s;R,t) \propto \frac{R^{d-1}}{|t-s|^{d/(2-\xi)}} \times \exp\left[-\text{const.}\frac{R^{2-\xi}}{|t-s|}\right] \qquad [23]$$

That confirms the diffusive character of the limiting process describing the Lagrangian trajectories in fixed non-Lipschitz velocities: the endpoints of the process stay at finite distance when the initial points converge. The PDF [23] changes from Gaussian to log–normal when ξ changes from 0 to 2. The Richardson dispersion $\langle R^2(t)\rangle \propto t^3$ is reproduced for $\xi = 4/3$.

Multiparticle Propagators

In studying multiparticle statistics, an important question is what memory of the initial configuration remains when final distances far exceed initial ones. To answer this question, one must analyze the conservation laws of turbulent diffusion. Many-particle evolution in nonsmooth velocities exhibits nontrivial statistical integrals of motion (martingales) that are proportional to the positive powers of the distances. The integrals involve geometry in such a way that the distance growth is balanced by the decrease of the shape fluctuations. The existence of multiparticle conservation laws indicates the presence of a long-time memory and is a reflection of the coupling among the particles due to the simple fact that they are all in the same velocity field. The conserved quantities may be easily built for the limiting cases. Already for a smooth velocity, the d-volume $\epsilon_{i_1 i_2 \ldots i_d} R_{12}^{i_1} \ldots R_{1d}^{i_d}$ is indeed preserved for $(d+1)$ Lagrangian trajectories. In the opposite case of a very irregular velocity, the fluid particles undergo a Brownian motion. The distances between the Brownian particles grow according to $\langle R_{nm}^2(t)\rangle = R_{nm}^2(0) + Dt$. The statistical integrals of motion are $\langle R_{nm}^2 - R_{pr}^2\rangle, \langle 2(d+2)R_{nm}^2 R_{pr}^2 - d(R_{nm}^4 + R_{pr}^4)\rangle$, and an infinity of similarly built harmonic polynomials (zero modes of Laplacian).

The statistics of the relative motion of N particles is described by the joint PDF averaged over rigid translations: $\mathcal{P}_N^{\mathrm{rel}}(\underline{r}, s; \underline{R}, t) = \int \mathcal{P}_N(s, \underline{r}; \underline{R} + \underline{\rho}, t)\, \mathrm{d}\rho$. For smooth velocities,

$$\mathcal{P}_N^{\mathrm{rel}}(\underline{r}, 0; \underline{R}, t) = \int \Big\langle \prod_{n=1}^{N} \delta(\boldsymbol{R}_n + \rho - W(t)\boldsymbol{r}_n) \Big\rangle \mathrm{d}\rho \qquad [24]$$

Such PDF depends only on the statistics of the evolution matrix $W(t)$ discussed earlier. Under the evolution governed by $W(t)$, all distances between points grow exponentially for large times while their ratios R_{nm}/R_{kl} tend to a constant. For whatever initial positions, asymptotically in time, the points tend to be situated on the line. Note that the existence of deterministic trajectories leads to the collapse property $\lim_{r_N \to r_{N-1}} \mathcal{P}_N^{\mathrm{rel}}(\underline{r}; \underline{R}; t) = \mathcal{P}_{N-1}^{\mathrm{rel}}(\underline{r}'; \underline{R}'; t)\, \delta(\boldsymbol{R}_{N-1} - \boldsymbol{R}_N)$, where $\underline{R}' = (\boldsymbol{R}_1, \ldots, \boldsymbol{R}_{N-1})$.

The long-time asymptotics of the propagators in the nonsmooth case can be found explicitly for the Kraichnan ensemble of velocities:

$$(\partial_t + M_N)\mathcal{P}_N^{\mathrm{rel}}(\underline{r}, s; \underline{R}, t) = \delta(t-s)\delta(\underline{R} - \underline{r}) \qquad [25]$$

$$M_N = \sum_{n<m} d^{ij}(\boldsymbol{r}_{nm}) \nabla_{r_n^i} \nabla_{r_m^j} \qquad [26]$$

When initial points get close or final points far apart and time gets large, the multiparticle PDF is factorized:

$$\lim_{\lambda \to 0} \mathcal{P}_N^{\mathrm{rel}}(\lambda \underline{r}, 0; \underline{R}, t) = \sum_{\beta} \lambda^{\zeta_\beta} f_\beta(\underline{r}) g_\beta(\underline{R}, t) \qquad [27]$$

where f_β must be taken as zero modes of $M_N^\dagger$ and its powers while $\partial_t g_\beta = -M_N g_\beta$. The remarkable feature of the zero modes of $M_N^\dagger$ is that they are conserved in mean by the Lagrangian evolution:

$$\partial_t \langle f(\underline{R}(t))\rangle = \int f(\underline{R}) M_N \mathcal{P}_N^{\mathrm{rel}}(\underline{r}, 0; \underline{R}, t)\, \mathrm{d}\underline{R}'$$
$$= \int \mathcal{P}_N^{\mathrm{rel}}(\underline{r}, 0; \underline{R}, t) M_N^\dagger f(\underline{R})\, \mathrm{d}\underline{R}' = 0$$

The scaling exponents of the zero modes depend, in a nontrivial way, on the number of particles N. For $\xi \ll 1$ and $d \gg 1$, one finds

$$\zeta_N = \frac{N}{2}(2-\xi) - \frac{N(N-2)}{2(d+2)}\xi \qquad [28]$$

Passive Scalar

For practical applications, for example, in the diffusion of pollution, the most relevant quantity is the average $\langle \theta(\boldsymbol{r}, t)\rangle$ which can be expressed via the single-particle propagator. As discussed earlier, for times longer than the Lagrangian correlation time, the particle diffuses and $\langle \theta \rangle$ obeys the effective heat equation

$$\partial_t \langle \theta(\boldsymbol{r}, t)\rangle = \left(D_{\mathrm{e}}^{ij} + \kappa \delta_{ij}\right) \nabla_i \nabla_j \langle \theta(\boldsymbol{r}, t)\rangle \qquad [29]$$

with the eddy diffusivity D_{e}^{ij} given by [11]. The simplest decay problem is that of a uniform scalar spot of size L released in the fluid. Its averaged spatial distribution at later times is given by the solution of [11] with the appropriate initial condition. On the other hand, the decay of the scalar in the spot is governed by the multipoint Lagrangian propagators. Taking the point of measurement inside the spot, consider the single-point moment $\langle \theta^N \rangle(t)$ described by [2]. If there is no molecular diffusion and the trajectories are unique (spatially smooth velocity), particles that end at the same

point remained together throughout the evolution and all the moments are preserved. On the contrary, when velocity is nonsmooth and the propagator is diffusive, we expect the decay even at the limit $\kappa \to 0$. This is an example of the so-called dissipative anomaly: the symmetry $t \to -t$ remains broken even when the symmetry-breaking factor κ goes to zero. Consider a spherical spot of θ released in a spatially smooth incompressible 3D flow with $\lambda_1 > \lambda_2 > 0 > \lambda_3$. During the time less than $t_d = |\lambda_3|^{-1} \ln (L/r_d)$, diffusion is unimportant and θ inside the spot does not change. At larger time, the dimensions of the spot with negative Lyapunov exponents are frozen at r_d, while the rest keep growing exponentially, resulting in an exponential growth of the total volume $\exp(\rho_1 + \rho_2)$. That leads to an exponential decay of scalar moments averaged over velocity statistics: $\langle [\theta(t)]^N \rangle \propto \exp(-\gamma_N t)$. The decay rates γ_N can be expressed via the PDF [18] of stretching variables ρ_i. Since θ decays as the inverse volume,

$$\langle [\theta(t)]^N \rangle \propto \int \mathrm{d}\rho_1 \mathrm{d}\rho_2 \exp[-tH(\rho_1/t - \lambda_1, \rho_2/t - \lambda_2) - N(\rho_1 + \rho_2)] \qquad [30]$$

At large t, the integral is determined by the saddle point. At small N, the saddle point lies within the parabolic domain of H so γ_N increases with N quadratically. At large N, the main contribution is due to the realization with smallest possible spot of size L so γ_N saturates.

For the decay in incompressible nonsmooth flow, using the Kraichnan model one gets

$$\langle \theta^{2n}(t) \rangle = \int \mathcal{P}_{2n}(\underline{0}; \underline{R}; -1)\, C_{2n}\left(t^{1/(2-\xi)}\underline{R}, 0\right) \mathrm{d}\underline{R} \qquad [31]$$

When $J_0 = \int C_2(\boldsymbol{r}, t)\,\mathrm{d}\boldsymbol{r} \neq 0$, the function $t^{d/(2-\xi)} C_2(t^{1/(2-\xi)}\boldsymbol{r}, 0)$ tends to $J_0\,\delta(\boldsymbol{r})$ in the long-time limit and [31] is reduced to

$$\langle \theta^{2n}(t) \rangle \approx (2n-1)!!\, J_0^n t^{nd/(\xi-2)} \times \int \mathcal{P}_{2n}(\underline{0}; \boldsymbol{R}_1, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_n, \boldsymbol{R}_n; -1)\,\mathrm{d}\underline{R} \qquad [32]$$

The decay is self-similar: $\mathcal{P}(t, \theta) = t^{d/2(2-\xi)} Q(t^{d/2(2-\xi)}\theta)$. That means that the PDF of $\theta/\sqrt{\bar{\epsilon}}$ is asymptotically time independent, with $\bar{\epsilon}(t) = \kappa \langle (\nabla\theta)^2 \rangle$ being time-dependent (decreasing) dissipation rate. This should be contrasted with the lack of self-similarity for the smooth case.

One can also consider steady state of θ pumped by a source $\phi(\boldsymbol{r}, t)$:

$$\partial_t \theta + (\boldsymbol{v} \cdot \nabla)\theta + \kappa \Delta \theta = \phi \qquad [33]$$

Assuming that pumping is white Gaussian with a zero mean and variance $\overline{\phi(\boldsymbol{r}_1, t_1)\phi(\boldsymbol{r}_2, t_2)} = \chi(\boldsymbol{r}_{12})\delta(t_2 - t_1)$, $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, one can express the correlation functions via the multiparticle propagators. For example, assuming zero conditions at the distant past and space homogeneity, one gets

$$C_2(\boldsymbol{r}, t) = \int_{-\infty}^{t} \mathrm{d}t' \int P(\boldsymbol{R}, \boldsymbol{r}, t')\chi(\boldsymbol{R})\,\mathrm{d}\boldsymbol{R} \qquad [34]$$

The function $\chi(\boldsymbol{R})$ is nonzero within the correlation scale L of the pumping which restricts integration to $R(t) < L$. For smooth velocity, this gives $F_2(r) = |\lambda_3|^{-1} \chi(0) \ln(L/r)$ at $r < L$. For nonsmooth velocity, the statistics of scalar fluctuations at small scales is described by the set of structure functions $S_N(r) \equiv \langle [\theta(r) - \theta(0)]^N \rangle \propto r^{\zeta_N}$ with the scaling exponents determined by the zero modes (see Falkovich *et al.* (2001)). Therefore, existence of Lagrangian statistical invariants explains the anomalous scaling of passive scalar (here, anomaly means that scale invariance broken by pumping is not restored even when the pumping scale goes to infinity).

See also: Anomalies; Intermittency in Turbulence; Large Deviations in Equilibrium Statistical Mechanics; Lyapunov Exponents and Strange Attractors; Random Walks in Random Environments; Stochastic Differential Equations; Turbulence Theories.

Further Reading

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Large Deviations in Equilibrium Statistical Mechanics

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Introduction

Large deviation theory (LDT) deals with the study of probabilities of extremely rare events. As an example, consider the case of independent identically distributed random variables $\sigma_1, \ldots, \sigma_N$ with the mean value $\mathbb{E}(\sigma_i) = m$. Then the typical deviations of the sum $M_N = \sigma_1 + \cdots + \sigma_N$ from its mean value Nm are of the order of $\sqrt{N}$, while in LDT we study the probabilities of the deviations which are linear in N. In "good" cases we know that for $b > 0$

$$\Pr\{M_N - Nm \geq bN\} \sim \exp\{-I(b)N\} \quad \text{as } N \to \infty \qquad [1]$$

where $I(\cdot) > 0$ is the "rate" function.

Questions of LDT are very natural in statistical mechanics, and they have deep physical meaning, notwithstanding the fact that the corresponding events are rare. One reason is that (some) rare events in the grand canonical ensemble become typical events in the canonical ensemble.

An interesting feature of LDT in statistical mechanics is that the behavior [1] of LD is not universal, and sometimes is replaced by a nonclassical one:

$$\Pr\{M_N - Nm \geq bN\} \sim \exp\{-\tilde{I}(b)N^{\nu}\} \qquad [2]$$

with $\nu < 1$. That usually happens in the "phase transition" regime, and then the quantity $\tilde{I}(b)$, as well as the exponent ν, have very much to do with the geometry of a droplet of one phase formed inside the other.

Below, we will illustrate all these features on the example of the Ising model.

The Ising Model in the Finite Box

Our random variables σ_x will take values ± 1, with $x \in \mathbb{Z}^d$. They are called spins. For every finite box $\Lambda \subset \mathbb{Z}^d$, we will define Gibbs states in Λ. To do this we need the Hamiltonians

$$H_{\Lambda,\xi}(\sigma) = -\sum_{\substack{x,y \text{ n.n.} \\ x,y \in \Lambda}} \sigma_x \sigma_y - \sum_{\substack{x,y \text{ n.n.} \\ x \in \Lambda, y \notin \Lambda}} \sigma_x \xi_y$$

Here, ξ is some spin configuration on $\mathbb{Z}^d$, which is called "boundary condition," while $\sigma \in \Omega_\Lambda$ is any spin configuration in Λ.

The "grand canonical Gibbs measure" $\mu_{\Lambda,\xi,T}$ in Λ with boundary condition ξ at inverse temperature $\beta = T^{-1}$ is given by

$$\mu_{\Lambda,\xi,T}(\sigma) = Z^{-1}_{\Lambda,\xi,T} \exp(-\beta H_{\Lambda,\xi}(\sigma)) \qquad [3]$$

where

$$Z_{\Lambda,\xi,T} = \sum_{\sigma \in \Omega_\Lambda} \exp(-\beta H_{\Lambda,\xi}(\sigma))$$

is called "partition function"; it makes the measure [3] to be a probability distribution.

The boundary condition $\xi \equiv +1(-1)$ will be denoted by $+(-)$. For every value of T, the Gibbs measures $\mu_{\Lambda(l),\pm,T}$ with $(\pm)$-boundary condition in the cubic box $\Lambda(l)$ of size l converge, as $l \to \infty$, to the probability measures that we will denote by $\mu_{\pm,T}$. If the two happen to be different, then $\mu_{+,T}$ is called the $(+)$-phase, and $\mu_{-,T}$ the $(-)$-phase. That happens to be the case iff the temperature T is lower than the critical temperature $T_c = T_c(d)$. The critical temperature depends on dimension; $T_c(1) = 0$, while $T_c(d) > 0$ for $d \geq 2$. The expectation

$$\mathbb{E}_{\mu_{+,T}}(\sigma_0) \equiv m(\beta)$$

is called spontaneous magnetization; $m(\beta) > 0$ iff $\beta > T_c^{-1}$.

LD Properties of the Gibbs States $\mu_{\Lambda(l),-,T}$

In what follows, we will discuss the LD properties of the sum $M_\Lambda = \sigma_1 + \cdots + \sigma_{|\Lambda|}$, where the spins σ_x, $x \in \Lambda$, are distributed according to the Gibbs state $\mu_{\Lambda,-,T}$. Note that $\mathbb{E}_{\mu_{-,T}}(\sigma_0) = -m(\beta)$.

Classical Case

If we look on the LDs of the sum M_Λ when the temperature T is high enough (in which case the limiting states $\mu_{+,T}$ and $\mu_{-,T}$ coincide), or else if the temperature is low, and the deviations are negative – that is, we consider the events $M_\Lambda + |\Lambda| m(T^{-1}) \leq b|\Lambda|$ with $b < 0$ – then their probabilities behave classically:

There exists a (high) temperature T_0 such that if $T > T_0$, then

$$\lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \Pr\{M_\Lambda + |\Lambda| m(T^{-1}) \leq b|\Lambda|\} = -I_T(b) \quad \text{for} \quad b \leq 0 \qquad [4]$$

$$\lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \Pr\{M_\Lambda + |\Lambda| m(T^{-1}) \geq b|\Lambda|\} = -I_T(b) \quad \text{for} \quad b \geq 0 \qquad [5]$$

where the function $I_T(b) \geq 0$ is strictly concave on the segment $(m(T^{-1}) - 1, m(T^{-1}) + 1)$. It vanishes at only one point $b = 0$.

There exists a (low) temperature T_1 such that if $T < T_1$, then the relation [4] holds with the function $I_T(b) > 0$ strictly concave on the segment $(m(T^{-1}) - 1, 0)$. The limit [5] also does exist, but it can vanish once we are in the phase transition region. In order to see some nontrivial behavior, we have to change the normalization $1/|\Lambda|$ in [5].

Nonclassical Case

The proper normalization happens to be the surface term, $1/|\Lambda|^{(d-1)/d}$:

There exists a temperature T_1 such that if $T < T_1$, then

$$\lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|^{(d-1)/d}} \Pr\{M_\Lambda + |\Lambda| m(T^{-1}) \geq b|\Lambda|\} = -\mathcal{W}_T(b) \quad \text{for} \quad b > 0 \qquad [6]$$

The function $\mathcal{W}_T(b)$ obeys $\mathcal{W}_T(b) = b^{(d-1)/d} w_T$, with $w_T > 0$, provided the value $b > 0$ is not too large: $b \leq b(d)$, where $b(d)$ is some constant, depending on the dimension and temperature; one can show that $b(d) \geq 1/2^d$. For larger b's the dependence is more complex.

The key object here is the constant w_T. To obtain it, one has to solve the following variational problem. Let $\tau_T(\theta)$, $\theta \in S^{d-1}$ be the surface tension between the (+)-phase and the (–)-phase of the Ising model at the temperature T. Then, for every closed compact (hyper)surface $M^{d-1} \subset \mathbb{R}^d$, we define its surface energy as

$$\mathcal{W}_T(M) = \int_M \tau_T(\theta_s)\, \mathrm{d}s$$

where θ_s is the normal vector to M at $s \in M$. The functional $\mathcal{W}_T(M)$ has the meaning of the energy of the M-shaped droplet of the (+)-phase floating in the (–)-phase. It is called the "Wulff functional." Let $\mathfrak{W}_T$ be the surface which minimizes $\mathcal{W}_T(\cdot)$ over all the surfaces enclosing the unit volume. Such a minimizer does exist and is unique up to translation. It is called the "Wulff shape." The value w_T is just the surface energy of the Wulff shape:

$$w_T = \mathcal{W}_T(\mathfrak{W}_T)$$

The value $b(d)$ is defined as the maximal value of b's, for which the dilatation $b^{1/d}\mathfrak{W}_T$ can fit into the unit cube. For higher values of b, the shape of the (+)-phase droplet in the cube with (–)-boundary condition is deformed by its walls, so its surface energy is given by a more complicated variational problem.

Moderate Deviations and the Droplet Condensation

The reason behind the different order of the probabilities of the events $M_\Lambda + |\Lambda| m(T^{-1}) \leq b|\Lambda|$, $b < 0$, and $M_\Lambda + |\Lambda| m(T^{-1}) \geq b|\Lambda|$, $b > 0$, at low temperatures is the following. A typical configuration contributing to the first event contains many small droplets of (–)-spins, of size $\leq \ln|\Lambda|$, floating in the sea of (+)-spins. On the contrary, in the case of the second event a typical configuration contains, in addition to small droplets, one large droplet of the size of Λ. It has a random shape, but in the limit $\Lambda \to \mathbb{Z}^d$ that shape converges to a nonrandom one, which happens to be the Wulff shape $\mathfrak{W}_T$. (The precise meaning of that statement depends on dimension; in case $d = 2$ the convergence holds in the Hausdorff metrics, while in higher dimensions it is known only in L^1 sense.) That statement makes the following question natural: consider the event

$$M_\Lambda - \mathbb{E}(M_\Lambda) \geq |\Lambda|^\alpha, \quad 0 < \alpha < 1$$

For which α should we expect, in addition to microscopic (+)-droplets of size $\leq \ln|\Lambda|$, the formation of a large droplet, of volume $\sim |\Lambda|^\alpha$, in a corresponding typical configuration? In other words, how many extra (+)-spins should we pump into our systems in order for the microscopic droplets to condense into a macroscopic one? (In the formulation of this question, we have to use the expectation $\mathbb{E}(M_\Lambda)$ instead of the asymptotically equivalent quantity $-|\Lambda| m(T^{-1})$. The difference, $\mathbb{E}(M_\Lambda) + |\Lambda| m(T^{-1}) \sim O(|\partial\Lambda|)$, being irrelevant in the LD case, becomes significant here.)

The answer is the following:

- if $\alpha < d/(d+1)$, then a typical configuration contains only microscopic droplets;
- if $\alpha > d/(d+1)$, then any typical configuration contains, in addition to microscopic droplets, one large droplet of volume $\sim |\Lambda|^\alpha$.

Therefore, the condensation happens at the value $\alpha = d/(d+1)$. This picture has its counterpart in the behavior of the probabilities of "moderate deviations" (MD), that is, events when $M_\Lambda + |\Lambda| m(T^{-1}) \geq |\Lambda|^\alpha$:

- if $\alpha < d/(d+1)$, then the deviation is due to independent fluctuations of sizes of many small droplets, and the usual Gaussian behavior holds:

$$\Pr\{M_\Lambda - \mathbb{E}(M_\Lambda) \geq |\Lambda|^\alpha\} \sim \exp\left\{-\frac{(|\Lambda|^\alpha)^2}{2\mathrm{Var}(M_\Lambda)}\right\} = \exp\left\{-c|\Lambda|^{2\alpha-1}\right\}$$

- if $\alpha > d/(d+1)$, then the deviation is due to the formation of a large droplet, and so

$$\Pr\{M_\Lambda - \mathbb{E}(M_\Lambda) \geq |\Lambda|^\alpha\} \sim \exp\left\{-c'|\Lambda|^{\alpha((d-1)/d)}\right\}$$

Note that the two estimates match at $\alpha = d/(d+1)$.

Other Questions

There are many related questions; some are partially solved, others are widely open, if considered on a rigorous mathematical level.

One can ask about the asymptotic behavior of probabilities of the events like

$$M_\Lambda - \mathbb{E}(M_\Lambda) = b_\Lambda$$

where the values b_Λ lie in the LD or MD region. The difference between such questions and those treated above is of the same nature as the difference between the integral and the local limit theorems. Partial answers to them are given in Dobrushin and Shlosman (1994).

Many results about the Wulff shape and its relation to the Ising model are known, starting by Dobrushin *et al.* (1992). Some are still challenging. One such question concerns the so-called roughening phase transition. It is known rigorously that the Wulff shape $\mathfrak{W}_T$ in the $d \geq 3$ Ising model has flat facets at low temperatures T. It is believed that such a feature holds true only for $T < T_R$, where the roughening temperature T_R is strictly less than the critical temperature $T_c(d)$ for $d = 3$. At the temperatures $T \in (T_R, T_c(3))$, the Wulff shape $\mathfrak{W}_T$ does not have facets. This conjecture seems to be very difficult.

The question about the typical behavior of the MD of the Ising model at the threshold value $M_\Lambda - \mathbb{E}(M_\Lambda) \sim |\Lambda|^{d/(d+1)}$ was recently answered in Biscup *et al.* (2003).

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Large-*N* and Topological Strings

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Introduction

Topological strings have been well studied since they were introduced in the early 1990s. Essentially, they are simplified string theories that capture the information about a sector of the full (or "physical") string theory. Thus, while sharing many of the structural features of usual string theory, they hold out the possibility of being amenable to explicit calculations. This is especially true with regard to stringy quantum corrections (the higher genus contributions from the point of view of the string world sheet), which are normally rather intractable in the full physical string theory. This has allowed them to play a useful role in enhancing the understanding of string theory and many of its mysterious quantum properties, such as the various dualities.

In particular, in the last several years, topological strings have served as an important laboratory for testing and understanding the connection between the large-N expansion of gauge theories and closed-string theories. In this article we will sketch how this connection is illustrated in a duality between large-N Chern–Simons gauge theory and closed topological string theories. We will survey the origin and current status of these developments and indicated some of its remarkable mathematical ramifications.

Background

In order to appreciate the conjecture relating the Chern–Simons theory and topological string theories, we need to go back to the seminal work of 't Hooft, who pointed to the connection between the large-N expansion of gauge field theories and string theories.

The starting point is a gauge field theory (with, say, gauge group U(N)), where we take the limit of the rank N of the gauge group to infinity (see Brezin

and Wadia (1993) for a collection of papers on the topic). The idea is then to make an expansion in inverse powers of N for various observables such as the free energy and correlation functions. For definiteness, let us take a gauge theory containing only gauge fields A in the adjoint representation of U(N). The quantum theory is (schematically) defined by the path integral

$$Z = \int [\mathcal{D}A] \mathrm{e}^{\mathrm{i}S(A)} \qquad [1]$$

For now, the action $S(A)$ for the gauge fields is left unspecified. It could be either the usual Yang–Mills functional or of the Chern–Simons form which we describe below. $S(A)$ is normalized in such a way that the gauge coupling constant, denoted by κ, only appears via an overall multiplicative factor of $1/\kappa$.

Then the expression, for instance, for the free energy $F = \ln Z$ has an expansion in a power series in κ, whose individual terms are given by the usual Feynman diagrammatic rules. Namely, we have is a sum over connected vacuum diagrams (those without any external legs) formed from the vertices determined by the action $S(A)$. Even without going into the details of the action, we can write down the dependence on N and κ coming from a diagram with h faces, V vertices, and E edges. Every edge is associated with a propagator (arising from the inverse of the quadratic term in $S(A)$) and thus comes with a weight of κ. Every vertex, coming from the cubic and higher-order terms in $S(A)$, comes with a factor of κ^{-1}. There is a factor of N coming from summing over the color indices that circulate in every loop (face). We thus get a weight of $N^h \kappa^{E-V}$ and so the total contribution to the free energy can be organized as

$$\begin{aligned} F &= \sum_{g=0,h=1}^{\infty} C_{g,h} N^h \kappa^{2g-2+h} \\ &= \sum_{g=0,h=1}^{\infty} C_{g,h} N^{2-2g} \lambda^{2g-2+h} \end{aligned} \qquad [2]$$

Here we have defined $\lambda \equiv \kappa N$, the 't Hooft coupling, as the combination that will be kept fixed when taking the limit of large N. We have also used the fact that $V - E + h = 2 - 2g$, where g is the number of handles of the closed two-dimensional surface one can associate with the Feynman diagram. (It is best to visualize the Feynman diagram as a "fatgraph" which forms the skeleton of a closed Riemann surface.) The coefficients $C_{g,h}$ represent the sum of the contributions from all genus g diagrams with h boundaries and depend on the details of the theory.

We note that the reorganization of the contributions to the free energy is reminiscent of the genus expansion in a string theory. In fact, eqn [2] as it stands looks like an open-string expansion on world sheets with g handles and h boundaries. Indeed, in many cases the gauge theory arises as a limit of an open-string theory. (Recall that a massless nonabelian gauge boson is one of the low-lying excitations of an open-string theory.) So the double expansion in terms of g and h is not too surprising.

However, the interesting conjecture of 't Hooft is in the relation to closed-string theory. Note that the expansion in inverse powers of N depends only on the number of handles g. In fact, $1/N$ seems to play the role of closed-string coupling in that it suppresses higher genus diagrams. The total contribution to a given genus g comes from summing over all the holes h in eqn [2], for example,

$$F = \sum_{g=0}^{\infty} N^{2-2g} F_g(\lambda) \qquad [3]$$

The conjecture is to identify this with a closed-string expansion in which $F_g(\lambda)$ is a closed-string amplitude on a genus g Riemann surface. (In carrying out the sum over the holes, we have assumed the existence of a radius of convergence. This is plausible since the number of planar diagrams ($g = 0$), for instance, grows only exponentially with the number of holes.) The question, since 't Hooft, has been: what is this closed-string theory? In other words, what is the background on which the closed string propagates?

A breakthrough came from Maldacena's identification of the background for the particular case of U(N) $\mathcal{N} = 4$ supersymmetric Yang–Mills theory. His conjecture was that this theory is dual to type IIB closed-string theory on $\mathrm{AdS}_5 \times S^5$ with a curvature scale set by λ and with closed-string coupling $\propto \lambda/N$. This proposal passed a number of nontrivial checks and is widely held to be true. It also stimulated the search for closed-string duals to other large-N gauge theories.

In what follows, we explain how the conjecture of 't Hooft has a nice realization in the case of three-dimensional U(N) Chern–Simons gauge theory on S^3. The dual closed-string theory, obtained by summing over the holes, turns out to be the A-model topological string on the (six-dimensional) resolved conifold background. The parameter λ maps into a Kahler parameter in the closed-string

geometry and once again the closed-string coupling is $\propto \lambda/N$.

The Large-*N* Expansion of Chern–Simons Theory

Nonabelian Chern–Simons theory is based on the following action functional for the U(*N*) gauge connection *A*:

$$S_{\mathrm{CS}}(A) = \frac{k}{4\pi}\int_M \mathrm{tr}\left(A \wedge \mathrm{d}A + \tfrac{2}{3} A \wedge A \wedge A\right) \qquad [4]$$

Here *M* is a three-dimensional manifold. *k* is called the level and is integer quantized for the path-integral equation [1] to be single valued. Note that, classically, κ as defined earlier is proportional to $1/k$. One of the nice properties of $S_{\mathrm{CS}}(A)$ is that it is independent of the metric on *M*, unlike the Yang–Mills functional. Thus, it is a prototype of a topological field theory. In fact, the observables in this theory capture topological information about the 3-manifold *M*.

Witten succeeded in quantizing the Chern–Simons theory by relating its Hilbert space to the space of conformal blocks in the two-dimensional U(*N*) WZW theory. (for more details on the quantization, *see* Chern-Simons Models: Rigorous Results). Here, merely the answers for various observables in the theory will be quoted. In particular, the free energy for the theory on S^3 can be written in a completely explicit form:

$$\begin{aligned} Z(S^3, N, k) &= \exp F(S^3, N, k) \\ &= \frac{1}{(N+k)^{N/2}} \prod_{j=1}^{N-1} \left(2 \sin \frac{j\pi}{N+k}\right)^{N-j} \end{aligned} \qquad [5]$$

One of the features one observes in the quantization is the shift ("finite renormalization") of the effective level from k to $k+N$. This can also be seen in perturbation theory. Consequently, while taking the large-*N* limit, the natural quantity to be held fixed as the 't Hooft coupling is $\lambda = 2\pi N/(k+N)$.

We can then carry out the 't Hooft expansion in powers of λ and $1/N$, of expressions, for example, for the free energy in eqn [5]:

$$\begin{aligned} F &= \frac{N^2}{2}\left(\log \lambda - \frac{3}{2}\right) - \frac{1}{12}\log N + \zeta'(-1) \\ &+ \sum_{g=2}^{\infty} \frac{1}{N^{2g-2}} \frac{B_{2g}}{2g(2g-2)} \\ &+ \sum_{g=0}^{\infty} \sum_{h=2}^{\infty} F_{g,h} \lambda^{2g-2+h} \end{aligned} \qquad [6]$$

The coefficents $F_{g,h}$ are nonzero only for even h and are given by

$$\begin{aligned} F_{0,h} &= -\frac{2\zeta(h-2)}{(2\pi)^{h-2}(h-2)h(h-1)} \\ F_{1,h} &= \frac{\zeta(h)}{6(2\pi)^h h} \\ F_{g,h} &= \frac{2\zeta(2g-2+h)}{(2\pi)^{2g-2+h}} \binom{2g-3+h}{h} \\ &\times \frac{B_{2g}}{2g(2g-2)} \end{aligned} \qquad [7]$$

where the last line is for $g > 1$. B_{2g} are the Bernoulli numbers. The first few terms in eqn [6] are nonperturbative contributions which do not have a Feynman-diagram interpretation. The power series in λ is, on the other hand, of the same form as eqn [2]. In fact, there is an open-string interpretation for these terms which will be considered later.

Given the explicit form of the answer, we can carry out the summation over the holes h. Using some resummation techniques, we find

$$F = \sum_{g=0}^{\infty} \left(-\mathrm{i}\frac{t}{N}\right)^{2g-2} F_g(t) \qquad [8]$$

with $t \equiv \mathrm{i}\lambda$ and

$$\begin{aligned} F_g(t) &= \frac{(-1)^g |B_{2g} B_{2g-2}|}{2g(2g-2)(2g-2)!} \\ &+ \frac{|B_{2g}|}{2g(2g-2)!} \sum_{n=1}^{\infty} n^{2g-3} \mathrm{e}^{-nt} \end{aligned} \qquad [9]$$

(This expression is for $g > 1$. There are very similar expressions for genus 0 and 1 as well.) With the identification of the string coupling $g_s = -\mathrm{i}t/N$, the $F_g(t)$ actually turn out to be the genus g amplitudes of a closed topological string, in line with the general expectation of the previous section. This is explained in the following.

Topological Strings

Physical strings are defined in terms of a two-dimensional sigma model (the theory on the world sheet) made reparametrization invariant by coupling to two-dimensional gravity. Topological strings are simpler versions of this, where the world-sheet theory is a two-dimensional topological sigma model. The latter is defined in terms of a sigma model (usually with $N=2$ superconformal symmetry) with an additional twist which drastically cuts down the physical states to a subset of the low-lying modes. There are actually two inequivalent twists

denoted by A and B, respectively, but we will restrict to the A twist in this article. One of the simplifications of the A twisted sigma model is that the path integral localizes to contributions from only holomorphic maps from the world sheet to the target space (which will be taken to be a Calabi–Yau 3-fold). Also, all the observables in the theory depend only on the Kahler parameters of the target space and not the complex structure parameters (*see* Topological Sigma Models as well as the book by Hori *et al.* (2003) for more details).

The topological string theory is defined by an appropriate integration of the observables of the topological sigma model over the moduli space of the world-sheet Riemann surface. For instance, the free energy of the string theory at genus g is given by

$$F_g^{\text{top}}(t) = \int_{\mathcal{M}_g} < \prod_{i=1}^{6g-6} (b, \mu_i) >_X \qquad [10]$$

Here b is one of the reparametrization ghost fields on the world sheet and μ_i are Beltrami differentials. The averaging is with respect to the world-sheet sigma model for the Calabi–Yau target X, as the subscript indicates. We have also shown the dependence of F_g on the Kahler parameters of X, collectively denoted by t. The localization to the holomorphic maps in the path integral implies that $F_g^{\text{top}}(t)$ takes the generic form

$$F_g^{\text{top}}(t) = \sum_\beta N_{g,\beta} q^\beta \qquad q^\beta \equiv \prod_i q_i^{n_i} \qquad [11]$$

Here $q_i = \mathrm{e}^{-t_i}$ and n_i are the integer coefficents labeling the element $\beta \in H^2(X)$. This is in the same basis of two cycles of $H^2(X)$ in terms of which the complex Kahler parameters t_i are expressed. (Recall that in string theory the Kahler parameters are complexified because of the presence of an additional 2-form field.) The $N_{g,\beta}$ are the Gromov–Witten invariants for X and are in general rational numbers. For nonzero β, the corresponding terms are often called world-sheet instanton contributions since they correspond to topologically nontrivial maps from the world sheet to 2-cycles in the target space. The all-genus free energy of the topological string is also defined to be

$$F^{\text{top}}(t, g_s) = \sum_{g=0}^{\infty} g_s^{2g-2} F_g^{\text{top}}(t) \qquad [12]$$

with g_s being the string coupling.

Since topological strings are related to physical strings by a twist on the world sheet, it is natural that topological string computations are related to computations in the physical string theory. In fact, as shown by Antoniadis, Gava, Narain, and Taylor as well as Bershadsky, Cecotti, Ooguri, and Vafa, observables such as $F_g^{\text{top}}(t)$ are related to special superpotential terms in the type II string compactification on the Calabi–Yau X. Using duality to M-theory, these answers were reinterpreted by Gopakumar and Vafa in terms of contributions coming from BPS states of wrapped D-branes. This gives a completely different perspective on topological strings. For instance, the all-genus free energy can naturally be reorganized as

$$F^{\text{top}}(t, g_s) = \sum_{g=0}^{\infty} \sum_\beta \sum_{d=1}^{\infty} n_\beta^g \frac{1}{d} \left(2 \sin \frac{d g_s}{2}\right)^{2g-2} q^{d\beta} \qquad [13]$$

where the n_β^g are integer invariants (Gopakumar–Vafa) since they count the number of BPS states. This will prove to be useful in extracting all-genus answers for topological string amplitudes, which is normally quite difficult using the perturbative definition given earlier.

The Large-N Dual to Chern–Simons Theory

We are now in a position to state the duality (Gopakumar and Vafa 1999) between large-N Chern–Simons theory and topological strings in a precise way. The conjecture is that the closed topological string theory on the S^2 resolved conifold geometry is exactly dual to the U(N) Chern–Simons theory on S^3. The resolved conifold geometry is a noncompact Calabi–Yau 3-fold described by the equation

$$xy - zw = 0 \qquad [14]$$

where the singularity is resolved by a 2-sphere $x = \rho z$, $w = \rho y$. The resulting space can thus be characterized as an $O(-1) + O(-1)$ bundle over P^1. It has a single Kahler parameter t for the nontrivial 2-cycle of the S^2. In addition, the string theory is characterized by the string coupling g_s. These parameters map on the gauge theory side to the 't Hooft parameter λ and N via the dictionary

$$t = \mathrm{i}\lambda, \qquad g_s = \frac{\lambda}{N} \qquad [15]$$

This conjecture can be checked by comparing various exact calculations in the Chern–Simons theory with corresponding calculations in the topological string on this conifold background. The use of the duality to M-theory enables us to make exact computations on this side as well. One of the

nontrivial checks of this duality comes from a comparison of the free energies. In eqns [8] and [9], we already have carried out the sum over the holes in the Chern–Simons theory and organized it as a closed-string genus expansion. Note that these expressions are already of the form [11] expected of a closed topological string. One simply has to check that it is indeed that on the S^2 resolved conifold.

In the language of the integer invariants n^g_β, the S^2 resolved conifold is particularly simple. The only nonzero invariant is $n^0_1 = 1$. Physically, this corresponds to a single brane wrapped on the genus-zero S^2. Putting this into eqn [13], and making the expansion in powers of g_s, we find exactly eqn [9] for the genus-g contribution to the free energy. This is quite a remarkable agreement and represents a triumph for the ideas of large-N duality.

Geometric Transitions and Large-*N* Duality

To understand the reason for this duality a bit better, we utilize an old observation of Witten that Chern–Simons theory is an open topological string theory. As mentioned earlier, the expansion [2] (or [6]) is suggestive of an open-string expansion in terms of handles and holes. Witten observed that open topological strings on the noncompact 3-fold T^*M (with Dirichlet boundary conditions on M for the end points of the string) is Chern–Simons theory on M. In fact, in the modern language of D-branes, we would say that U(N) Chern–Simons theory is the world-volume theory of N D-branes wrapped on M, for the topological A-model on T^*M.

In particular, Chern–Simons theory on S^3 is the theory of branes wrapped on S^3 inside T^*S^3. The latter is the conifold geometry but now deformed by a nonzero size S^3. It is described by the equation

$$xy - zw = \mu \qquad [16]$$

where μ is the deformation which parametrizes the size of the S^3.

The above large-N duality can be considered as an open–closed string duality. Namely, that the theory of open A-model topological strings on the S^3 resolved conifold (with N D-branes) is dual to closed A-model topological strings on the S^2 resolved conifold. Cast in this way, we see that the duality involves a transition in the background geometry in going from the open-string to the closed-string description. The sum over the holes changes the background. The S^3, as it were, shrinks to zero size and a transverse S^2 opens up. This geometric transition makes the connection between the Chern–Simons theory and the closed topological string somewhat less mysterious. Maldacena's conjecture for super Yang–Mills involves a similar passage from D-branes in flat space to a closed-string theory on anti-de Sitter space. In fact, it appears as if the best way to understand 't Hooft's idea in generality is to think of it as an open–closed string duality.

Further Checks and Consequences

The free energy is not the only gauge-invariant observable in Chern–Simons theory. One important class of observables, which played an important role in the connection with knot invariants, are the Wilson loop expectation values. Given a knot $\mathcal{K}$ in S^3, we can define, in terms of an arbitrary representation R of U(N), the trace of the holonomy around the knot averaged with respect to the Chern–Simons path-integral measure:

$$W_R(\mathcal{K}) = < \mathrm{tr}_R\left(P\exp \mathrm{i}\oint_{\mathcal{K}} A\right) > \qquad [17]$$

P denotes path ordering. Similarly, we can also define the expectation values of links: products of traces of holonomies around various interlinked paths. The nonperturbative solution of Chern–Simons theory gives exact answers for the expectation values of these Wilson loops. The discussion below is, however, confined to knots.

Since the trace of holonomies is being considered in different representations, it makes sense to study the generating functional

$$Z(U,V) = \sum_R \mathrm{tr}_R(U)\mathrm{tr}_R(V) = \exp\left[\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{tr}\ U^n \mathrm{tr} V^n\right] \qquad [18]$$

The source V here is a U(M) matrix, unrelated to the U(N) holonomy U around $\mathcal{K}$. The second equality in [18] follows from use of the Frobenius formula. It was shown by Ooguri and Vafa that this generating functional is the natural object from the point of view of the open–closed string duality.

We have already mentioned that the U(N) Chern–Simons theory can be thought of as the theory of N topological D-branes wrapped on the Lagrangian S^3 cycle inside T^*S^3. For a knot $\mathcal{K}$ in the S^3, we consider another Lagrangian 3-cycle $\hat{C}_{\mathcal{K}}$ in T^*S^3 which intersects the S^3 exactly in $\mathcal{K}$. A canonical construction for $\hat{C}_{\mathcal{K}}$ is

$$\hat{C}_{\mathcal{K}} = \left\{(q(s),p) \in T^*S^3 | \sum_i p_i\dot{q}_i = 0\right\} \qquad [19]$$

where the knot $\mathcal{K}$ is parametrized by the closed curve $q(s)$. By construction, $\hat{C}_{\mathcal{K}}$ intersects the S^3 in $\mathcal{K}$. Now consider M D-branes wrapped on $\hat{C}_{\mathcal{K}}$. One now has to consider the fields coming from the strings stretching between the two sets of branes. One can show that integrating out these fields (which are in the bifundamental of the product group $U(N) \times U(M)$) modifies the original Chern–Simons action to

$$S_{\text{eff}}(A) = S_{\text{CS}}(A) + \sum_{n=1}^{\infty} \frac{1}{n} \text{tr}U^n \text{tr}V^n \qquad [20]$$

Here V is the holonomy around $\mathcal{K}$ of the $U(M)$ gauge field $\tilde{A}$. Thus, this configuration of M probe branes gives rise exactly to the generating function eqn [18] for Wilson loops of $\mathcal{K}$.

The geometric transition which relates the Chern–Simons theory to the closed-string theory now suggests what one needs to do to compute this generating function on the closed-string side. We have to follow the configuration of the M probe branes on $\hat{C}_{\mathcal{K}}$ through the conifold transition in which the S^3 shrinks and one blows up the S^2. It is not easy in general to figure out the Lagrangian cycle $C_{\mathcal{K}}$ which results from following $\hat{C}_{\mathcal{K}}$ through the transition. It has only been done in a class of knots including the simple unknot. But assuming we know $C_{\mathcal{K}}$, the generating function for Wilson loops is given by the free energy on the S^2 resolved conifold in the presence of M probe branes on $C_{\mathcal{K}}$. This requires one to know more than the closed-string partition function computed earlier. We now also need to compute amplitudes for world sheets with boundary on $C_{\mathcal{K}}$. These are called open-string Gromov–Witten invariants and the study of this subject is in its infancy. For simple knots such as the unknot, for which $C_{\mathcal{K}}$ is known, these can be computed. One finds again a remarkable agreement with the nonperturbative answers of Chern–Simons theory. Thus, the computation of knot invariants gets related to open-string Gromov–Witten invariants. There have been a number of other tests involving more general knots and links. One also has to be careful of subtleties such as in the choice of framing. The reader is referred to the articles by Marino (2002, 2004) for these topics.

Conclusions

The large-N duality of 't Hooft is realized in Chern–Simons theory in a very explicit way. Thanks to the analytic control we have over both Chern–Simons theory as well as closed topological strings, the conjecture passes very nontrivial checks that extend to all-genus case. This is more than we can do in the AdS/CFT conjecture where most computations are at tree level in the supergravity limit. In contrast, here we see the essential stringiness of the closed-string dual to Chern–Simons theory.

Also, by viewing it as an open–closed string duality, many aspects of the correspondence were clarified. It, therefore, provides a useful toy model for a general understanding of open–closed string duality. Indeed, a proof of this duality using world sheet techniques has been proposed by Ooguri and Vafa. One would like to carry over some of the intuition that operates in this duality to the case of other physically interesting gauge theories.

From the mathematical point of view, as already indicated, this duality leads to previously unsuspected relations between Gromov–Witten invariants and invariants of 3-manifolds, including those of knots. In fact, by considering more general geometric transitions and using this duality locally, one can learn about all-genus topological string amplitudes for a wide class of noncompact toric geometries. This line of development culminated in the formulation of the topological vertex by Aganagic, Klemm, Marino, and Vafa, which captures the essence of the topological closed-string amplitudes for noncompact toric geometries. As in the case of the general correspondence between the gauge theory and gravity, this duality sheds new light on both sides of the equation. We learn to see new integrality properties in knot and 3-manifold invariants which have an interpretation in terms of enumerative problems in 3-folds. The surprises that such a deep connection presages have not yet been exhausted.

See also: AdS/CFT Correspondence; Chern–Simons Models: Rigorous Results; Duality in Topological Quantum Field Theory; Free Probability Theory; The Jones Polynomial; Knot Theory and Physics; Large-*N* Dualities; Quantum 3-Manifold Invariants; Schwarz-Type Topological Quantum Field Theory; String Field Theory; Topological Gravity, Two-Dimensional; Topological Quantum Field Theory: Overview.

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Large-N Dualities

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Introduction

Gopakumar and Vafa (1999) conjectured that U(N) Chern–Simons gauge theory on S^3 is dual, for large values of N, to a closed topological string theory on a suitable Calabi–Yau 3-fold X. They suggested that this duality is realized by a geometric "transition," a topological surgery which can be realized by birational contractions followed by the complex deformations of Calabi–Yau varieties. Here we will give some general comments on the history of this conjecture and then present some of its mathematical implications; we will focus on the geometric transition and the novel mathematics that it has generated.

A duality relating gauge theories and string theories (with gravity) was first conjectured by 't Hooft (1974). In 1998 Maldacena conjectured a duality between Yang–Mills gauge theory with $N=4$ SUSY on a four-dimensional manifold M and IIB type closed string on the anti-de Sitter space $\mathrm{AdS}^5 \times S^5$. Chern–Simons string theory is a three-dimensional theory and purely topological, hence it is in principle simpler than four-dimensional Yang–Mills theory, which also involves a metric.

In this survey, we discuss the IIA open/closed dualities: we will mostly be concerned with the partition function, that is we will be working in the context of "topological strings." The duality has been extended to a duality of strings, adding fluxes on the closed sector and branes on the open sector. There is much mathematical evidence supporting the conjecture.

Overview

The conjecture says that U(N) Chern–Simons gauge theory on S^3 is dual, for large values of N, to type IIA closed topological string theory on a suitable Calabi–Yau manifold X. A starting point for the geometry, and its mathematical implications, is that S^3 can be thought of as a vanishing cycle in a local Calabi–Yau manifold $Y = T^*S^3$, which deforms to a singular Calabi–Yau Y_0; X is a Calabi–Yau birational resolution of Y_0. X are Y are related by a geometric transition. In fact, Witten showed that quantum Chern–Simons theory on S^3 can be thought of as open IIA (with U(N) branes) on $Y = T^*S^3$; thus, a more general conjecture says, loosely speaking, that open IIA theory on a Calabi–Yau manifold Y is dual, for large N, to closed IIA on a Calabi–Yau X which is related to Y via a geometric transition. A consequence of a physics "duality" is a matching of the free energies of the dual theories. In this particular case, if the conjecture is true, the Chern–Simons free energy $Z(S^3, \mathrm{U}(N))$ should determine, and be determined by, the closed prepotential $\mathcal{F}_{\mathrm{cl}}(X,t)$. Note that $Z(S^3, \mathrm{U}(N))$ is purely topological, and that $\mathcal{F}_{\mathrm{cl}}(X,t)$ includes all genera, as we will discuss later. A mathematical application is computing Gromov–Witten invariants for higher genus via large-N dualities (Mariño 2004). Another consequence involves the matching of the observable in S^3 and X.

This conjecture is now supported by a vast amount of evidence. Vafa, Gopakumar and Ooguri noted, via a string-theory analysis, that topological and knot invariants of S^3 (computed through U(N) Chern–Simons theory on S^3) determine and are determined by, for large N, the Gromov–Witten invariants of X in a neighborhood of the exceptional locus of the birational contraction $X \rightarrow Y_0$.

The extension to the full string theory would say that open string of type IIA compactified on a Calabi–Yau manifold Y with branes is conjectured to be dual to closed string of type IIA compactified on a Calabi–Yau manifold X with fluxes, if X and Y are related by a geometric transition.

A mathematical consequence of this statement is that the closed Gromov–Witten invariants of X agree, with a suitable identification of the parameters, with combinations of open Gromov–Witten invariants and knot invariants of Y. This has been shown to hold for some classes of examples.

This circle of ideas has stimulated much work in physics and mathematics on the nature of the mathematical correspondence behind this duality, as well as the property of the enumerative and topological invariants involved. The "mirrors" of the above transitions have been studied in a series of papers, starting with the work of Dijkgraaf and Vafa (2002).

The mathematics behind the open/closed dualities is still not understood: it is reasonable to speculate that the natural setup is a framework of symplectic field theory.

We shall start by discussing the principal topics of this large-N duality: Chern–Simons quantum field theory, IIA closed prepotential (and Gromov–Witten invariants), and Chern–Simons as open string (and IIA open prepotential). Next we shall study the geometric transitions and conclude with some mathematical predictions of the duality.

We shall not discuss some other interesting implications of this duality. For example, we shall not discuss its mirror IIB duality: it is known that the part of the closed prepotential in IIA corresponding to rational curves can be expressed as its IIB mirror dual with periods over certain suitable cycles; the IIA open contribution corresponding to open discs is expressed in terms of integrals over chains and the Abel–Jacobi map. We only remark that this large-N duality has also been interpreted as a duality between seven-dimensional manifolds with G_2 holonomy.

History

The chronology of various important contributions in the field of large-N duality is as follows:

- 1976: 't Hooft's conjecture
- 1988: Clemens introduces transitions
- 1988: Witten introduces quantum Chern–Simons theory on 3-manifolds
- 1992: Witten discusses Chern–Simons theory as open string
- 1998: Gopakumar–Vafa–Ooguri
- 2001: Verification for unknot, Katz–Liu, Li, and Song
- 2001: Lift to manifolds with G_2 holonomy
- 2002: The conjecture verified for many examples of conifold transitions, including compact case; the topological vertex is introduced
- 2003: Relations with Donaldson–Thomas invariants

Background

The varieties of interest in the physical theory must satisfy certain "supersymmetry" conditions; in particular, a complex algebraic manifold is required to be Calabi–Yau, a real seven-dimensional Riemannian manifold is required to have G_2 holonomy group. Also of particular interest are the Lagrangian real submanifolds of the Calabi–Yau 3-folds. By a Calabi–Yau manifold X we mean a manifold with $c_1(X)=0, h^0(\Omega^k)=0$, where Ω^k is the sheaf of holomorphic k-forms, and $0<k<\dim(X)$. If $\dim X\geq 2$, we also assume that X is simply connected, but not necessarily compact. For example, if $\dim(X)=1$, X is a torus, if $\dim(X)=2$, X is a $K3$ surface, if $\dim(X)\geq 3$, X is simply called a Calabi–Yau manifold. A compact Kähler manifold (M,g,J) of complex dimension $m\geq 3$ is a Calabi–Yau variety if and only if its holonomy is $\mathrm{SU}(m)$. A subvariety L of a symplectic manifold (X,ω) is Lagrangian if $\omega_{|\mathrm{L}}=0$ and $\dim L=(1/2)\dim X$. Sometimes we consider noncompact manifolds, thought of as neighborhoods of a compact projective Calabi–Yau manifold. Typically, our symplectic manifold is a Calabi–Yau 3-fold (X,ω) together with its Kähler form ω. If there exists an antiholomorphic involution, then the fixed locus is a Lagrangian submanifold.

The Dualities

We will take the point of view that dualities in physics imply relations between geometric invariants, without dwelling on the physics of the dualities themselves. A consequence of a physics "duality" is the matching of the prepotential of two dual string theories.

A Few Comments on Chern–Simons Theory: Free Energy (Partition Function)

Let L be a closed oriented manifold together with a principal G-bundle. The classical Chern–Simons action is defined as $S(L,A)=\int_L\alpha(A)$, where α is a 3-form on L which depends on a connection A and a suitable bilinear invariant form on the Lie algebra $\mathfrak{g}$. It is well defined under gauge transformations modulo the integers; $\mathrm{e}^{2\pi \mathrm{i}S(L,A)}$ is well defined. In the large-N dualities considered here, the groups of interests are $\mathrm{SU}(N)$ and $\mathrm{U}(N)$. The first check of the duality was found with $G=\mathrm{SU}(N)$ and $M=S^3$; later it was discovered that the correct group for the matching of the observables must be $\mathrm{U}(N)$, while both can be used for the free energies. We shall consider $G=\mathrm{SU}(N)$ and $M=S^3$. Without loss of generality, the bundle can be taken to be the product $\mathrm{U}(N)\times S^3$; any bilinear invariant form on the Lie algebra $\mathfrak{su}(N)$ is necessarily an integer multiple k of the Cartan–Killing form on the Lie algebra. Then $S=S(k,A)$ and

$$S(k,A)=-\frac{k}{8\pi^2}\int_{S^3}\mathrm{tr}\left(A\wedge \mathrm{d}A+\tfrac{2}{3}A\wedge A\wedge A\right)$$

where k is the "level" of the theory. Witten defines the quantum Chern–Simons theory by taking the integral of the Chern–Simons action over all possible connections $\mathcal{A}$ modulo gauge equivalence $\mathcal{G}$:

$$\begin{aligned}Z(S^3,\mathrm{SU}(N))&=\int_{\mathcal{A}/\mathcal{G}}(D\mathcal{A})\mathrm{e}^{2\pi\mathrm{i}S(A)}\\&=\int_{\mathcal{A}/\mathcal{G}}(D\mathcal{A})\exp\left(-\frac{k\mathrm{i}}{4\pi}\int_{S^3}\mathrm{tr}\left(A\wedge\mathrm{d}A+\tfrac{2}{3}A\wedge A\wedge A\right)\right)\end{aligned}$$

Witten shows how to calculate the free energy $Z(S^3,\mathrm{SU}(N))$ through topological surgery, assuming $Z(S^2\times S^1)=1$. Witten also defines the partition

function of knots and links in L (the "expectation values"), which are knot and link invariants. The expectation values are computed by evaluating the trace of the holonomy transformation of a $U(N)$ connection around the knot, and then taking a suitable average of the $U(N)$ connections. These invariants depend on a choice of the framing of the knot (or link).

The explicit computations involve physics, representation theory, and topology. If $L = S^3$, then:

$$Z(S^3, SU(N)) = (k+N)^{-N/2}\sqrt{\frac{k+N}{N}} \times \prod_{j=1}^{N-1}\left\{2\sin\left(\frac{j\pi}{k+N}\right)\right\}^{N-j}$$

Reshetikin and Turaev, among others, described mathematically the Chern–Simons free energy and the expectation values.

A Few Comments on Closed-String Theory: Free Energy (Prepotential)

In IIA closed-string theory on X, a Calabi–Yau manifold, one considers holomorphic stable maps of closed Riemann surfaces of genus $g, \phi : \Sigma_g \to X$, with $\phi_*(\Sigma_g) = [\beta] \in H_2(X, \mathbb{Z})$, for all genera g and homology classes $\beta \in H_2(X, \mathbb{Z})$.

Then one forms the closed prepotential $\mathcal{F}_{cl}(X, t)$, which encodes the enumerative invariants of such maps to X, and which depends on the Kähler parameters t of X. Sometimes the prepotential is also called "free energy" in the physics literature or Gromov–Witten prepotential, as it contains the Gromov–Witten invariants of X. Setting $\mathcal{F}_g(q) = \sum_{\beta \in H_2(X,\mathbb{Z})} C_{g,\beta} q^\beta$, the closed prepotential is defined as

$$\mathcal{F}_{cl}(X, q) = \sum_{g>0}^{\infty} g_s^{2g-2}\mathcal{F}_g(q)$$

Here q is a formal variable such that $q^{\beta_1+\beta_2} = q_1^\beta \cdot q_2^\beta$ (for $\beta_1, \beta_2 \in H_2(X, \mathbb{Z})$) and g_s is the string coupling constant. $C_{g,\beta}$ are the genus g Gromov–Witten invariants of X, corresponding to the class β and they have been defined as

$$C_{g,\beta} = \int_{[\overline{M}_{g,0}(X,\beta)]^{\text{virt}}} 1$$

It is difficult to explicitly compute the invariants $C_{g,\beta}$; in particular, there is no known general method for calculating these invariants. They are computed mostly via "localization" methods, in the presence of a suitable torus action. In the case of $g = 0$ the invariants are often computed via IIA–IIB duality, calculating certain periods in the mirror manifold W.

Example (Faber–Pandharipande). Let $X \cong \mathcal{O}_{\mathbb{P}^1}(-1) \oplus \mathcal{O}_{\mathbb{P}^1}(-1)$; X is a neighborhood of a rigid rational curve, which can be thought of as a local Calabi–Yau manifold; then all the effective curves $\beta \in H_2(X, \mathbb{Z})$ must be of the form $\beta = d[\mathbb{P}^1]$, $\forall d \in \mathbb{N}$. Faber and Pandharipande showed that

$$\mathcal{F}_{cl}(X, q) = \sum_{d=1}^{\infty} \frac{q^d}{2\sin(dg_s/2)^2} \qquad [1]$$

This formula was proved with localization methods after it was conjectured by Gopakumar and Vafa using large-N dualities. In fact, a consequence of a duality between two theories is the matching of the free energies of two dual string theories. In this particular case, the conjectures imply that Chern–Simons free energy determines, and is determined by, the all-genus closed prepotential of a suitable Calabi–Yau manifold X:

$$Z(S^3, U(N)) \rightleftarrows \mathcal{F}_{cl}(X, t)$$

Note that the left-hand side is purely topological, as we saw in the previous section, while the right-hand side is holomorphic.

The *trait d'union* between the two prepotentials is given by the interpretation of Chern–Simons theory on S^3 as open-string theory on T^*S^3 and the geometric transition.

A Few Comments on Open-String Theory with Branes: Open Prepotential

Let Y be a Calabi–Yau manifold together with $\{\cup L_i\}$, Lagrangian submanifolds; to each submanifold L_i is assigned a gauge group $G_i : L_i$ is wrapped with G_i-branes. Here we shall focus on the case $G_i = U(N_i)$ and we will write $(Y; L_i, U(N_i))$.

Witten shows that the open prepotential $\mathcal{F}_{op}(Y, \lambda, t_{op}, g_s)$ depends on 't Hooft's coupling constants λ_i associated to Chern–Simons theory on the Lagrangian submanifolds $(L_i, U(N_i))$, together with the open Kähler parameters $t_{op} \in H_2(X; \cup L_i, \mathbb{Z})$, and the string coupling constant g_s. To describe the open prepotential, Witten argues, we consider all maps of Riemann surfaces with boundary to Y, with the condition that the boundaries are mapped to the Lagrangian submanifolds L_i; one should also include all the "highly degenerate holomorphic maps," in particular those which contract $\Sigma_{g,h}$ to a "ribbon graph" on the Lagrangian $\cup L_i$. The contribution of these highly degenerate maps is captured by the quantum Chern–Simons theory of the Lagrangians $\{L_i, U(N_i)\}$.

Application 1 (Chern–Simons free energy as open prepotential). Let us consider open IIA on $Y = T^*S^3$ with U(N)-branes wrapped on $L = S^3$: L is a Lagrangian submanifold with the standard symplectic structure; note that in T^*L there are no nontrivial homology curves. Then, according to Witten, the corresponding open prepotential $\mathcal{F}_{\text{op}}(Y, \cup L_i)$ must only depend on the "highly degenerate" maps and must consist of the Chern–Simons term F_{CS} on $L = S^3$. In particular,

$$F_{\text{CS}} = \log Z(S^3) = \mathcal{F}_{\text{op}}(Y, \lambda, g_s)$$

where $\lambda = 2N\pi/(k+N)$ is the 't Hooft coupling constant. Periwal (1993) showed that, for large N, $\log Z(S^3)$ could be expanded as a closed-string expansion:

$$F_{\text{CS}}(\lambda) = \sum_{g \geq 0} \mathcal{F}_g(\lambda) g_s^{2\,2g}$$

where $g_s =: 2\pi/(k+N)$ is the Chern–Simons coupling constant. In 1998 Gopakumar and Vafa, using physics arguments, deduced that the expansion would have the closed form [1], which was later proved by Faber and Pandharipande.

The explicit description of the open prepotential in the presence of homology classes is not known; one would need to combine the enumerative invariants of open maps together with the quantum Chern–Simons factor. We shall discuss an approach at the end of this note, but consider first the geometric transition.

The Transition

The conjecture says that $U(N)$ Chern–Simons gauge theory on S^3 is dual, for large values of N, to IIA closed topological string theory on a suitable Calabi–Yau manifold X. A starting point to find such X is that S^3 is a Lagrangian 3-cycle in the manifold $Y = T^*S^3$; performing a topological surgery by replacing S^3 with S^2 one obtains a (local) Calabi–Yau manifold X, on which the dual IIA theory is compactified. The key observation is that Y can be identified with the algebraic variety of equation $\{xy - zw = t\} \subset \mathbb{C}^4$ and that this is a complex smoothing (in fact the Milnor fiber) of Y_0 with equation $\{xy - zw = 0\} \subset \mathbb{C}^4$. On the other hand, X is a small resolution of this singularity, where $\mathbb{P}^1$ is the exceptional locus of the birational contraction. The origin is an "ordinary double point" singularity and the nontrivial sphere $S^3 \subset Y$ is the vanishing cycle of the degeneration. The manifolds involved are noncompact: the exceptional curve $[\mathbb{P}^1] = t$ is the only nontrivial homology class in X, and the enumerative invariants in X can be thought as the contribution of the exceptional curve in a neighborhood of a Calabi–Yau manifold. We shall present the steps leading to this construction and the evidence for the conjecture.

The Local Construction of *X*

Let $Y_\mu = \{(w_1, \ldots, w_4) \in \mathbb{C}^4$ such that $\sum_{j=1}^4 w_j^2 = \mu\}$.

Proposition 1 *Let μ be a nonzero real positive parameter; then:*

- $L = S^3 \subset T^*S^3$ *is a Lagrangian submanifold of* T^*S^3 *with its standard symplectic structure;*
- $T^*S^3 \cong Y_\mu$ *and* $L \cong L_\mu \overset{\text{def}}{=} \{\text{Re}(\sum_{j=1}^4 w_j^2 = \mu)\}$.

In fact, we can embed T^*S^3 in $\mathbb{R}^8$ as

$$\sum_{j=1}^4 q_j^2 = 1, \qquad \sum_{j=1}^4 q_j p_j = 0$$

where $S^3 = \{p_i = 0\}$; consider then the morphism $\mathbb{C}^4 \to \mathbb{R}^8$ defined by setting

$$q_j = \frac{\text{Re}(w_j)}{\sqrt{\mu + \sum_i v_i^2}}, \qquad p_j = \text{Im}(w_j)$$

which induces the diffeomorphism $Y_\mu \cong T^*S^3$ of the statement.

Remark 1 Let $Y_0 = \{\sum_{j=1}^4 w_j^2 = 0\} \subset \mathbb{C}^4$; then:

- Y_0 is singular at the origin,
- Y_μ is a complex deformation of Y_0, and
- L_μ is called a "vanishing cycle."

With a change of coordinates we can write the equation of Y_μ as $\{xy - zw = 0\}$; the singularity is still at the origin. This singularity is an ordinary double point, which is often referred in physics literature as "the conifold singularity." Let $X \subset \mathbb{C}^4 \times \mathbb{P}^1$ be defined:

$$\lambda z + \nu y = 0, \qquad \lambda x + \nu w = 0$$

$[\lambda, \nu] \in \mathbb{P}^1$.

Remark 2 X is smooth and the morphism

$$\phi : X \longrightarrow Y_0, \quad ((x, y, z, w), [\lambda, \mu]) \mapsto (x, y, z, w)$$

is an isomorphism $\phi_{|_{X\setminus\mathbb{P}^1}} : (X \setminus \mathbb{P}^1) \simeq (Y_0 \setminus \{0\})$ and $\mathbb{P}^1 \mapsto (0, 0, 0, 0,) \subset \mathbb{C}^4$. ϕ is a small (nondivisorial) birational resolution of the singularity at the origin. Y_μ is a deformation (smoothing) of Y_0. Note that topologically $S^3 \cong L_\mu \subset Y_\mu$ has been replaced by $\mathbb{P}^1 \cong S^2 \subset X$. The algebraic properties of the topological surgery between Y_μ and X were first studied by Clemens in 1988.

Transitions in Geometry

A transition between X and Y is a birational contraction from a smooth Calabi–Yau X to a singular variety Y_0 followed by a complex deformation to another smooth Calabi–Yau manifold Y:

$$\begin{array}{ccc} & & X \\ & & \downarrow \\ Y & \leftsquigarrow & Y_0 \end{array}$$

The vanishing cycles of the complex deformation $\cup L_i$ are always Lagrangian submanifolds of Y. The transition makes sense if $\dim(X) = \dim(Y) \geq 2$ and it is nontrivial if $\dim(X) = \dim(Y) \geq 3$, when the topology of X is different from the topology of Y. The possible transitions among Calabi–Yau 3-folds have been classified.

Conjecture 1 Let X and Y be Calabi–Yau manifolds related by a geometric transition: then IIA open theory with $U(U)$ branes compactified on $(Y, \cup L_i)$ is dual to IIA closed theory compactified on X (with fluxes).

As a consequence:

Conjecture 2 Let X and Y be Calabi–Yau manifolds related by a geometric transition: then $\mathcal{F}_{\mathrm{op}}(Y, \lambda, g_s, t_{\mathrm{op}}) = \mathcal{F}_{\mathrm{cl}}(X, q, g_s)$ for a suitable identification of the parameters.

The results stated in the previous section can be summarized in the the following statement, which is the proof of the above conjecture for the special case of a local conifold transition:

Theorem 1 *Let* $X \cong \mathcal{O}_{\mathbb{P}^1}(-1) \oplus \mathcal{O}_{\mathbb{P}^1}(-1)$ *and* $Y = T^*S^3$ *with* $U(N)$ *branes wrapped on* $L = S^3$. *Then* X *and* Y *are related by a conifold transition and* $\log F_{CS}(S^3) = \mathcal{F}_{\mathrm{op}}(Y, \lambda) = \mathcal{F}_{\mathrm{cl}}(X, q)$, *with the identification*

$$\lambda = \frac{2N\pi}{k+N} = q, \qquad g_s = \frac{2\pi}{k+N}$$

This matching of the free energies is supporting evidence for the large-N conjecture. At this moment, we still do not know if Conjectures 1 and 2 hold for more general transitions.

A Few Comments on Knots and Links

Later, Ooguri and Vafa extended the conjecture to the observables, that is, by adding knots and links in S^3; the guiding principle is that a knot (or link) $\mathcal{C} \subset S^3$ should determine a noncompact Lagrangian submanifold $\mathcal{L}_\mathcal{C} \subset X$; it is conjectured that the knot (and link) invariants, expressed as expectation values, should determine and be determined by the enumerative invariants of morphisms of bounded Riemann surfaces, with boundaries mapped onto $\mathcal{L}_\mathcal{C}$. We refer to these invariants as open Gromov–Witten invariants. While both statements have been verified with mathematical techniques only when $\mathcal{C}$ is the unknot, there is much supporting evidence for the conjecture in general. We will not describe these aspects here but only make a few remarks.

The expectation values of a knot $\mathcal{C}$ are computed by taking first the trace of a holonomy matrix of a $U(N)$ connection A along $\mathcal{C}$ and then integrating over all connections (modulo gauge equivalence). As for the case of the Chern–Simons free energy, the definition of expectation values has been worked out both in the realm of physics and of mathematics. The expectation values are knot and link invariants, and depend on a choice of the framing of the knot (or link). The open Gromov–Witten invariants have not yet been constructed, as we shall discuss in the following section; however, starting with the work of Katz and Liu, Li and Song open invariants have been successfully calculated in the presence of a torus action. The resulting invariants do depend on the choice of the torus action, which has been shown to match the choice of the framing of the knot (or link).

More on the Open Prepotential

The open Gromov–Witten invariants, in analogy with the closed case, should "count" in an appropriate sense open morphisms; at this point, it is not known how to define this quantity. To proceed in analogy with the closed case, one would need to define the appropriate moduli space of open maps and its virtual fundamental class. On the other hand, open invariants have been successfully calculated in the presence of a torus action, assuming the existence of the moduli and virtual fundamental class and that the Atiyah–Bott localization theorems can be applied. We shall follow this approach in sketching how the IIA prepotential has been computed in many examples.

Open Invariants

Let $[\beta] \in H_2(Y; \cup L_i, \mathbb{Z})$ be the relative homology class of Riemann surfaces in Y with boundary on the union of the Lagrangian 3-cycles $\cup_i L_i$ and a class $[\gamma] \in H_1(\cup L_i)$.

If $\Sigma_{g,h}$ is a Riemann surface of genus g and h boundary components, let $\phi : \Sigma_{g,h} \to Y$ be a morphism with

$$\phi_*(\Sigma_{g,h}) = [\beta] \in H_2(Y; \cup L_i, \mathbb{Z})$$

The open generating function is

$$F_o(Y, \cup L_i, t_{\text{op}}, g_s) = \sum_{g,h\geq 0}^{\infty} g_s^{2g-2+h} F_{g,h}(t_{\text{op}})$$

with

$$F_{g,h}(t_{\text{op}}) = \sum_{\beta,\gamma} C_{g,h,\beta,\gamma} q^{\beta} y^{\gamma}$$

Here q and y are formal variables such that $q^{\beta_1+\beta_2} = q^{\beta_1} \cdot q^{\beta_2}$ and $y^{b_1+b_2} = y^{b_1} \cdot y^{b_2}$, for $\beta_1, \beta_2 \in H_2(Y; \cup L_i, \mathbb{Z}), \gamma_1, \gamma_2 \in H_1(\cup L_i, \mathbb{Z})$; t_{op} is the open Kähler parameter, g_s is the string coupling constant and $C_{g,h,\beta,\gamma}$ should "count" in an appropriate sense the maps ϕ.

Example (Ooguri–Vafa; Katz–Liu; Li–Song). If $Y = \mathcal{O}_{\mathbb{P}_1}(-1) \oplus \mathcal{O}_{\mathbb{P}_1}(-1)$, then t is the class of the $\mathbb{P}^1 \cong S^2$, $t/2$ represents the class of the lower hemisphere in S^2. The Lagrangian L is the Lagrangian $\mathcal{L}$ in the previous sections, which corresponds to the unknot in $S^3 \subset Y$; it is the fixed locus of an antiholomorphic involution on X and it intersects S^2 in an equator. Then, for a suitable choice of the torus action:

$$F_o(Y, \cup L_i, t_{\text{op}}, g_s) = \sum_d \frac{y^d}{2d \sin(d\lambda/2)} \mathrm{e}^{-dt/2}$$

There is a complete form for more general torus actions. The above formula was first computed by Ooguri and Vafa, using string-theory arguments, and then computed by the mathematicians, Katz and Liu, and Li and Song.

More on the Open IIA Prepotential

If there is only one rigid open curve in Y, say a disk C, with boundary on $L \subset Y$, then, as Witten showed, the open prepotential is a combination of the open enumerative invariants as described above with $\beta = d[C]$ and $\gamma = \partial C$ and the expectation values of the unknot ∂C. The variable Y is changed in the trace of the holonomy of a connection.

In the presence of a torus action, one can treat the fixed locus as if it were rigid and proceed accordingly.

With these techniques, Conjecture 2 has been verified for many cases of conifold transitions, with t_{op} nontrivial, for a suitable identifications of the parameters, including when both X and Y are compact manifolds (Diaconescu–Florea 2003).

See also: AdS/CFT Correspondence; Chern–Simons Models: Rigorous Results; Large-*N* and Topological Strings; Mirror Symmetry: A Geometric Survey; String Field Theory.

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Lattice Gauge Theory

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Introduction

As a prototype of lattice gauge theory, quantum chromodynamics (QCD) will be considered in this article. All statements about QCD can easily be extended to other theories, with different gauge group and different content of particles.

QCD is a gauge theory with gauge group SU(3) (color group), coupled to spin-1/2 particles (quarks) belonging to the fundamental representation of the color group. There exist in Nature six different species (flavors) of quarks, with masses ranging from $m_{\text{up}} \sim 5\,\text{MeV}$ to $m_{\text{top}} \sim 180\,\text{GeV}$: the values of these masses are determined by other interactions and can be treated as input parameters of the theory as well as the number of quark flavors. In standard notation, the Lagrangian reads

$$L = -\frac{1}{2}\text{tr}(G_{\mu\nu}G_{\mu\nu}) + \sum_f \bar{\psi}_f(\text{i}\not{D} - m_f)\psi_f \qquad [1]$$

The sum runs over the six quark flavors f. $G_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\nu + \text{ig}[A_\mu, A_\nu]$ is the field strength tensor, $A_\mu = \sum T^a A^a_\mu$ the (gluon) gauge field, $T^a(a = 1, \ldots, 8)$ are the eight generators of the gauge group in the fundamental representation, normalized as $\text{tr}(T^a T^b) = (1/2)\delta^{ab}$. ψ_f is a color triplet of fields. Under a gauge transformation $U(x)$,

$$\psi_f(x) \to \psi'_f(x) = U(x)\psi_f(x) \qquad [2]$$

$$A_\mu(x) \to A'_\mu(x) = U(x)A_\mu U^\dagger(x) + \text{i}U(x)\partial_\mu U^\dagger(x) \qquad [3]$$

D_μ is the covariant derivative of ψ

$$D_\mu\psi_f = (\partial_\mu - \text{ig}A_\mu)\psi_f \qquad [4]$$

and transforms like ψ_f by construction.

L is invariant under the gauge transformation equations [2] and [3]. As a consequence of gauge invariance, the theory has one single coupling constant g.

To make connection with the observations, one has to solve the theory, that is, one has to construct a Hilbert space on which the fields act as operators obeying the equations of motion and the canonical commutation relations. In textbook field theory, this is done by splitting the Lagrangian L into two parts:

$$L = L_0 + L_\text{I} \qquad [5]$$

with L_0 the part of L which is bilinear in the fields and L_I the rest. L_0 can be solved exactly since it describes free particles and the corresponding equations of motion are linear. The resulting Hilbert space is the Fock space of free particles. L_I is treated as a perturbation producing scattering between the fundamental particles. This approach works well in quantum electrodynamics, where the observed particles (electrons and photons) coincide with the excitations of the fundamental fields of the Lagrangian.

In QCD, the fundamental excitations (the quarks and the gluons) are observed as particles neither in Nature nor as a product of high-energy collisions between elementary particles. This feature is known as confinement of color. The conjecture is that excitations with nontrivial color are forbidden to propagate as free particles. However, if hadrons are probed at short distances by photons or by leptons, everything works as if they were composite states of quarks. The accepted explanation relies on asymptotic freedom: the effective coupling constant becomes small at short distances (high momentum transfers) and the constituents behave as free particles.

At large distances, the fundamental excitations are not observed, the interaction is strong and the perturbative picture describing scattering between quarks and gluons is not adequate for the real world.

An alternative quantization procedure is needed which does not rely on perturbation theory. A formally exact quantization procedure is the Feynman path integral. The solution of the theory is given in terms of a functional integral $Z[J]$, which generates the correlators of the fields in the ground state (vacuum). Indicating symbolically the Lagrangian coordinates, namely the fields, by a single symbol Φ, one has

$$Z[J] = \int \prod_x \text{d}\Phi(x) \exp\left[-S[\Phi] - \int J(x)\Phi(x)\text{d}x\right] \qquad [6]$$

The connected Euclidean vacuum correlators are given in terms of functional derivatives of $Z[J]$

$$< 0|T(\Phi(x_1)\Phi(x_2)\cdots\Phi(x_n))|0 >_{\text{conn}} = \frac{1}{Z[0]}\frac{\delta^n Z[J]}{\delta J(x_1)\delta J(x_2)\cdots\delta J(x_n)}\bigg|_{J(x)=0} \qquad [7]$$

"Euclidean" means that they are analytic continuations to imaginary times. Going to Euclidean system is necessary to isolate the vacuum state. The amplitudes can be analytically continued back to Minkowski space. The Hilbert space and all the physical observables can be constructed in terms of the correlators, a property known as reconstruction theorem. Formally (i.e., assuming that everything makes sense only if the functional integral exists),

$$\begin{aligned}&< 0|T(\Phi(x_1)\Phi(x_2)\cdots\Phi(x_n))|0 >_{\text{conn}}\\&= \frac{1}{Z}\int\prod_x \mathrm{d}\Phi(x)\\&\times \exp(-S[\Phi])\Phi(x_1)\Phi(x_2)\cdots\Phi(x_n)\end{aligned} \qquad [8]$$

The continuation to imaginary time changes sign to the kinetic energy, and Z formally becomes the partition function of a four-dimensional statistical model with Hamiltonian $S_{\mathrm{E}}[\Phi]$, a general fact in Feynman integrals.

By definition of functional integral, Z is defined by discretizing a finite volume V of spacetime to a finite set of points and then sending their number to infinity, making a set dense in V. If the limit exists, a Z_V is obtained. The volume V is then sent to infinity, to cover the whole spacetime (thermodynamical limit) and Z_V eventually converges to Z. A rigorous proof of the existence of these limits does not exist for QCD, but there are qualitative arguments that this is the case, which will be presented below.

In the lattice formulation of field theory, a regular lattice, usually cubic, is taken as a discretization of spacetime.

From the very definition of Feynman integral, it follows that the formulation of field theory on the lattice is nothing but an approximation to the limit which defines Z. It will provide a good approximation if the lattice spacing is small enough with respect to the physical lengths involved and if the lattice is large compared to them.

Perturbation theory amounts to split the action into a bilinear term S_0 and an interaction term S_{I} containing the higher powers of the fields. The Z integral is then computed by expanding the weight in a power series of S_{I}:

$$\begin{aligned}&\int\prod_x \mathrm{d}\Phi(x)\exp(-S_0 - S_{\mathrm{I}})\\&= \int\prod_x \mathrm{d}\Phi(x)\exp(-S_0)\sum_n \frac{(-S_{\mathrm{I}})^n}{n!}\end{aligned} \qquad [9]$$

The Feynman integral thus becomes Gaussian, can be computed, and gives the usual perturbative expansion. The two limits (integral and series expansion) do not commute in general. For QCD, there are indeed arguments that the renormalized perturbative expansion does not converge and is plagued by singularities known as renormalons.

Wilson's Formulation

For field theories of scalar particles, the lattice discretization is performed by assigning a value of the field to each site of the lattice. The Wilson formulation for gauge theories is not made in terms of the fields A_μ, which are defined in the Lie algebra of the gauge group, but in terms of parallel transports, which are elements of the group itself. The building blocks are parallel transports along links parallel to spacetime axes connecting neighboring sites

$$\begin{aligned}&U_\mu(x)\\&\equiv P\exp\left(\mathrm{i}g\int_x^{x+\hat{\mu}} A_\rho \mathrm{d}x^\rho\right) \approx \exp(\mathrm{i}gaA_\mu(x))\end{aligned} \qquad [10]$$

where $\hat{\mu}$ indicates the vector of length a in the μ direction and P the ordered product. The last approximate equality is valid in the limit of small lattice spacing a. g is the coupling constant.

Under a gauge transformation $V(x)$,

$$U_\mu(x) \to V(x)U_\mu(x)V^\dagger(x+\hat{\mu}) \qquad [11]$$

It follows from eqn [11] that the parallel transport along a closed path is gauge invariant. The density of action can be written in terms of the parallel transport along the elementary square of links in the hyperplanes $\mu\nu$ $\Pi_{\mu\nu}$, known as plaquette:

$$\prod_{\mu\nu} = \mathrm{tr}[U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x)] \qquad [12]$$

By expanding in powers of a, one easily finds

$$\prod_{\mu\nu} = N_{\mathrm{c}} - \frac{1}{2}a^4\mathrm{tr}[G_{\mu\nu}G_{\mu\nu}] + O(a^6) \qquad [13]$$

with N_{c} the number of colors, 3 for QCD. The lattice action can be defined as

$$S = \sum_{x\mu\nu}\beta\left(1 - \frac{1}{N_{\mathrm{c}}}\Pi_{\mu\nu}\right) \qquad [14]$$

with $\beta = 2N_{\mathrm{c}}/g^2$, and tends to the continuum action as $a \to 0$, $O(a^2)$. An infinite number of higher-order terms in a exist, which come from the expansion of the links, but they are expected to be irrelevant in the continuum limit $a \to 0$.

The measure of the Feynman integral is assumed to be the Haar measure of the gauge group for each link, which again can be shown to tend to the continuum measure in the continuum limit.

Everything is gauge invariant, contrary to the perturbative formulation, where a gauge fixing is required to define the vector meson propagator.

By Weierstrass theorem, the integral is finite for any finite number of links, the gauge group being compact.

Any other choice of the lattice action differing from the Wilson action of eqn [14] by terms of higher order in a will have the same continuum limit: there is significant freedom in the choice of the action.

In the language of statistical mechanics, the Euclidean lattice formulation is a spin model. Different choices of the action correspond to different spin models. In the vicinity of a second-order phase transition, however, the correlation length becomes large with respect to the lattice spacing and all the irrelevant terms become negligible. All the spin models at the critical point belong to the same universality class and define the same field theory.

This is what happens for QCD because of asymptotic freedom. By renormalization group arguments, the lattice spacing behaves as

$$a(\beta) \approx \frac{1}{\Lambda}\exp(-b_0\beta) \qquad [15]$$

at sufficiently large β, where $-b_0$ is the coefficient of lowest-order term of the β-function, b_0 is positive and Λ is a physical scale. As $\beta \to \infty$, a tends exponentially to zero in physical units and the coarse structure of the lattice becomes unimportant, indicating that the short-distance limit in the definition of the Feynman integral exists. The theory also develops a mass scale Λ which insures the existence of a finite correlation length and hence of the thermodynamical limit. In practice, when β is increased, the lattice space becomes exponentially small in physical units. As a consequence, however, the physical scale becomes exponentially large in lattice units, and an exponentially large lattice is needed to insure the large-distance convergence. This makes life difficult if the Feynman integral has to be computed numerically.

Quarks

Fermion fields are defined on lattice sites. The naive lattice transcription of the fermion term in eqn [1] consists in replacing the covariant derivatives by finite differences with parallel transports to make the result gauge covariant. In principle, $D_\mu\psi(x) = U^\dagger(x)\psi(x+\hat{\mu}) - \psi(x)$ is a correct definition. In practice, a more symmetric difference is used which is correct $O(a^2)$, namely

$$D^{\mathrm{L}}_\mu\psi(x) = \frac{1}{2}[U(x)\psi(x+\hat{\mu}) - U^\dagger(x-\hat{\mu})\psi(x-\hat{\mu})] \qquad [16]$$

The fermionic Lagrangian then reads

$$\sum_x \bar{\psi}(x)[\mathrm{i}\not{D}^{\mathrm{L}} - m]\psi(x) \equiv \sum_{x,x'\alpha\beta} \bar{\psi}_\alpha(x)M^{-1}_{\alpha\beta(x,x')}\psi_\beta(x') \qquad [17]$$

It is convenient to indicate this expression in the form $S_f = \bar{\psi}M^{-1}\psi$, where ψ is a large column whose elements are labeled by the site x and by the component α. The functional integral over ψ can explicitly be done by using the standard rules of integration on Grassman variables, since the action is bilinear,

$$Z = \int \prod \mathrm{d}U_\mu(x)\mathrm{d}\psi(x)\mathrm{d}\bar{\psi}(x) \times \exp(-S_{\mathrm{E}}[U] - \bar{\psi}M\psi) \qquad [18]$$

The result is

$$Z = \int \prod \mathrm{d}U_\mu(x)\exp(-S_{\mathrm{E}}[U])\det M \qquad [19]$$

The effect of fermions is to multiply the weight by a functional determinant which depends on the gauge field configuration.

A problem exists, however, in this procedure already at the level of free fermions, that is, putting $U=1$ in the action and in the determinant of eqn [18]. The equation of motion reads, in Fourier transform,

$$\sum_\mu \left[\gamma_\mu \sin\left(2\pi\frac{k_\mu}{L}\right) - m\right]\tilde{\psi}(k) = 0 \qquad [20]$$

With respect to the continuum, the momentum $p_\mu = 2\pi k_\mu/L$ has been replaced by its sinus. At small values of p_μ, eqn [20] coincides with the Dirac equation. However, an alternative solution exists at $p_\mu \approx \pi$, for each μ independently. The new equation differs from the other by a change of sign of γ_μ. Changing sign of one of the gammas means changing sign to $\gamma^5 \equiv \gamma^1\gamma^2\gamma^3\gamma^4_;$ which is the chirality of the fermion. Instead of one fermion, we then have $2^4 = 16$ fermion species, organized in pairs with opposite chiralities. It is impossible to have a single fermion with a given chirality. A number of recipes have been proposed to circumvent this artifact of the lattice regulation, for example, introduce by hand a term in the action which removes the spurious particles in the limit of zero lattice spacing (Wilson's fermions); double the lattice spacing by constructing two sublattices on even and odd sites, respectively, which propagate fermions of opposite chirality (staggered fermions),

so that the argument of the sinus in the derivative is doubled. More recently, an idea which goes back to Ginsparg and Wilson has been implemented, which consists in replacing a strictly local equation of motion like eqn [20] by an equation with the same continuum limit which is nonlocal, but with a nonlocality falling off exponentially at large distances, a recipe which makes propagation of chiral fermions possible. This is an important improvement, even if very demanding in computer power.

Numerical Simulations

Solving analytically the lattice version of QCD would allow one to follow constructively all the steps which bring to the definition of Z, that is, the ultraviolet and the infrared limit, as explained earlier. Presently that is out of reach. Also an attempt by Wilson to solve the lattice renormalization group equations by techniques of decimation is not conclusive.

The problem can be attacked numerically. One way would be to compute the integral numerically. That is, however, prohibitive: it would be like solving exactly the equations of motion for the molecules of a gas. The lattice theory is in fact a four-dimensional statistical mechanics with the Boltzmann factor $\beta = 2N_c/g^2$ and Hamiltonian equal to the Euclidean action. As in statistical mechanics the way out is to create a significant sample of configurations with weight $\exp(-\beta S_E)$ and to determine the field correlators which describe physics by an average on this ensemble. This is done by Monte Carlo techniques.

The basic principle is to start from an arbitrary field configuration and make a sequence of random changes, normally on a single link at a time, with uniform probability in the group measure so as to converge toward the equilibrium distribution $\exp(-\beta S_E)$. For that purpose, the probability $P_{C'C}$ to change from a configuration C to another C' is constrained to obey the detailed balance relation

$$P_{C'C} \exp(-\beta S[C]) = P_{CC'} \exp(-\beta S[C']) \qquad [21]$$

A common algorithm is known as metropolis. The way to implement the condition (eqn [21]) is to accept the new trial configuration C' if $S[C'] \leq S[C]$, and to accept it with probability $\exp(-\beta[S(C') - S(C)])$ if $S[C'] \geq S[C]$. An alternative method is known as "heat-bath". If the probability of the configuration for one link at a fixed value of the other variables is explicitly known, the change can be accepted with that probability.

In the presence of dynamical quarks, the integral eqn [18] is converted into an integral on bosonic variables by inverting the matrix M:

$$Z = \int \prod \mathrm{d}U_\mu(x)\, \mathrm{d}\phi(x)\, \mathrm{d}\phi(x)^\dagger \times \exp(-S_E[U] - \phi^\dagger [M^\dagger M]^{-1} \phi) \qquad [22]$$

The property has been used such that $\int \prod \mathrm{d}\phi(x)\, \mathrm{d}\phi^\dagger(x) \exp(-\phi^\dagger [M^\dagger M]^{-1} \phi) = |\det M|$. A metropolis updating is then performed on the combined U_μ and ϕ variables. To have a choice of the trial uniform in the measure, an algorithm is commonly used which is based on ergodicity, known as hybrid molecular dynamics. A fictitious conjugate momentum is associated with all variables, and a fictitious Hamiltonian is defined by adding to the action, considered as a potential energy, the sum of the squares of the conjugate momenta. A classical evolution is then performed in time by small steps which should displace the state in phase space ergodically: the evolution is called a trajectory. After a number of steps, a metropolis test is made as explained above.

Typically, the computer time needed to produce a significant configuration is proportional to the volume V of the lattice for pure gauge systems, to $V^{5/4}$ in the hybrid algorithm for full QCD.

As explained before, in order to have a good approximation to the Feynman integral the lattice spacing has to be small compared to the physical scales, for example, with respect to the Compton wavelength of the heaviest quark. On the other hand, to control volume effects it has to be large compared to the biggest physical length, for example, with respect to the Compton wavelength of the lightest quark. Since there is a factor $m_{\text{top}}/m_{\text{up}} \approx 3 \times 10^3$ between these two lengths, the lattice size needed would be prohibitive from numerical point of view. In practice, lattices of size L^4 are affordable with $L \leq 64 - 128$. For this reason, only the light quarks u, d, s are kept, which have mass smaller than the typical scale of the theory, which can be identified as the square root of the string tension. In the limit in which light quark masses are small compared to QCD scale, the Lagrangian is invariant under any unitary mixing of them. A global SU(3) invariance exists, which is known as flavor symmetry, and is broken by the difference of quark masses. Heavier quarks can be described by an effective theory, since they have negligible dynamical effects at low energies.

A Selection of Physics Results

String Tension

A big excitement followed the first numerical calculations by M Creutz at the beginning of the 1980s in which the static potential $V(r)$ between a quark and an antiquark was computed in pure-gauge theory on the lattice. One way to measure it is to measure the correlator of two Polyakov lines at a distance r on a significant ensemble of field configurations. The Polyakov line is the parallel transport in the fundamental representation along the time axis across the lattice: with periodic boundary conditions it is a closed loop, and hence it is gauge invariant. It can be proved that the log of this correlator is equal to $-V(r)aL_t$ with L_t the extension of the lattice in the time direction. It was found that

$$V(r) = \sigma r \qquad [23]$$

The parameter σ is known as string tension. A potential of the form eqn [23] means confinement: an infinite amount of energy is required to pull apart the particles at infinite distance. The parameter σ can be determined phenomenologically from the mass spectrum of the mesons and $\sigma 2\pi \approx 1\,\text{GeV}$. What is measured on the lattice is

$$\sigma a(\beta)^2 n^2 \qquad [24]$$

where n is the distance of the two Polyakov lines in lattice spacings and $a(\beta)$ the lattice spacing in physical units. In fact, the computer only produces pure numbers. If the lattice QCD belongs to the same universality class of QCD at the critical point, that is, if the lattice really defines QCD, the dependence of $a(\beta)$ on β is dictated by the β-function of the renormalization group. At sufficiently large $\beta = 6/g^2$,

$$a(\beta) \approx \frac{1}{\Lambda_{\text{latt}}} \exp(-b_0 \beta) \qquad [25]$$

with $b_0 = (11/3)N_c/16\pi^2$. Λ_{latt} is the energy scale of the theory. The measurement of the potential gives indeed a dependence of the lattice spacing on β consistent with eqn [25] and allows one to determine $\sigma/\Lambda^2_{\text{latt}}$. The absolute value of the lattice spacing can be determined by comparison with the physical value of the string tension. The theory is able to produce a physical scale. The correlation length is finite and as a consequence the infrared limit of the Feynman integral exists.

Mass Spectrum

Any operator with the quantum numbers of a particle can be used as interpolating field for it. The correlator of the operator at large distances behaves like a sum of exponentials $\exp(-mr)$ with m the masses of the particles with the same quantum numbers. At large distances the lightest particle dominates, especially if the operator has a good overlap, that is, if its matrix element between vacuum and the state of the particle is the biggest. From the correlators mr can be determined. On the lattice $r = na(\beta)$ so that, by eqn [25] what is really determined is the ratio m/Λ_{latt}. If Λ_{latt} has been determined, for example, from the string tension, the mass of the particle results in physical units. Alternatively, the ratios of any two masses can be determined and the scale fixed by the value of one of them. A good agreement is obtained already in pure gauge (quenched approximation) indicating that the quark loops are relevant at the level of 10% typically. This fact supports the idea that the large N_c-limit is a good approximation to reality, quark loops being nonleading in that limit. The light particle masses are more difficult to compute, being sensitive to the masses of light quarks which cannot be taken at realistic values due to computational difficulties: large lattices are required and big fluctuations are present near the chiral point. The spectrum of particles made of heavy quarks can be computed using effective theories, and nicely fits experiment. A byproduct is a precise determination of the gauge coupling constant, competitive with phenomenological determinations from short distance perturbative QCD.

Weak Interaction Matrix Elements

There exist matrix elements of currents (or products thereof) entering in weak amplitudes which involve large distances and are not computable in perturbation theory. Lattice can be used to evaluate them. Renormalization problems can appear in this approach when the cutoff is removed, which, however, are not difficulties of principle but only of technical nature. This activity is of fundamental importance to have precise predictions in order to understand the limits of the standard model.

Finite-Temperature QCD and the Deconfinement Transition

The static thermodynamics of a system of fields is described by the partition function

$$Z_T = \text{tr}[\exp(-H/T)] \qquad [26]$$

It is easy to show that Z_T is equal to the Euclidean Feynman integral on the imaginary time interval $(0, 1/T)$ with boundary conditions in time periodic for bosons and antiperiodic for fermions. Indeed, the

Boltzmann factor is formally an imaginary time evolution by $1/T$. A lattice of extension $L_t L_S^3$ with $L_s \gg L_t$ provides the partition function at a temperature $T = 1/aL_t$, if a is the lattice spacing in physical units.

Finite-temperature simulations are important to investigate the transition from the phase in which color is confined to a phase in which quarks and gluons can propagate as free particles. This phase is called deconfined phase or quark gluon plasma.

Big experiments at Brookhaven and at CERN are looking for this phase transition in high-energy collisions between heavy nuclei, but no definite evidence has yet been produced for it. Lattice simulations instead definitely prove that such a transition exists. For pure SU(3) gauge theory (quenched) at $T \approx 270\,\mathrm{MeV}$, a first-order phase transition is observed, at which the string tension vanishes. In a more realistic theory with dynamical quarks, a transition is also observed at $T \approx 160\,\mathrm{MeV}$, where chiral symmetry, which is spontaneously broken at zero temperature, is restored. This transition is also associated to deconfinement even if, in the presence of light quarks, the string tension does not exist. Indeed, when pulling apart a quark and an antiquark, an instability for production of quark–antiquark pairs sets in when the potential energy becomes large enough, which physically manifests itself as a production of light mesons. An alternative order parameter is needed. The possibility of defining alternative order parameters is discussed in next section.

The equation of state can also be studied relating internal energy to pressure, which is useful to understand heavy ion collisions.

From the features of the deconfinement transition, information can be extracted on the mechanisms by which QCD confines color.

A connected issue is the behavior of QCD at nonzero baryon density or chemical potential. The corresponding thermodynamics is described by a grand canonical ensemble

$$Z_\mu = \mathrm{tr}[\exp[-(H + \mu N)/T]] \qquad [27]$$

where $N = \int \mathrm{d}^3x \psi^\dagger \psi$ is the baryon number operator and μ the chemical potential. In the process of converting the partition function Z_μ into a Feynman integral, the term H at the exponent of eqn [27] generates the Euclidean action, which is real. The term proportional to N becomes imaginary. The integral is well defined, but the analogy with a four-dimensional statistical mechanics is broken, the effective Hamiltonian being non-Hermitian and no sampling can be made. Approximate methods have been developed, but the problem is open. Exploring numerically the region of phase space with $\mu \neq 0$ would be interesting, since a rich structure is expected, which could be relevant to dense systems such as neutron stars.

Mechanisms of Color Confinement

Understanding how QCD manages to confine color is one of the most fascinating problems in field theory.

To prove confinement, one should, in principle, prove that, at zero temperature, no gauge-invariant quasilocal operator exists, carrying nontrivial color and obeying cluster property at large distances. This proof is not known. There exists evidence form lattice simulations that a string tension exists, as discussed before. In any case, a guess can be made of the physical mechanism of confinement. If confinement is an absolute property reflecting a symmetry property of the vacuum, an order parameter should exist which discriminates between confined and deconfined phase, and the transition between the two phases has to be a true transition. Observing a crossover in some part of the boundary between the two phases would disprove this view. A lattice determination of the order of the deconfining transition is therefore of fundamental importance.

A possible mechanism of confinement proposed by G't Hooft is dual superconductivity of the vacuum: dual means interchange of electric with magnetic with respect to ordinary superconductors. In the same way as the magnetic field is constrained into Abrikosov flux tubes in an ordinary superconductor, the chromoelectric field acting between a quark and an antiquark would be constrained into flux tubes by a dual Meissner effect producing an energy proportional to the distance, or a string tension.

This mechanism can be investigated by lattice simulations, by checking if any magnetically charged operator exists whose vacuum expectation value is nonzero in the confined phase signaling condensation of magnetic charges and zero in the deconfined phase. Progress has been made in this direction which, however, is not yet conclusive. Chromoelectric flux tubes between q–$\bar{q}$ pairs are observed in lattice field configurations.

Topology

Euclidean QCD admits classical solutions with finite action and with a nontrivial topology which makes them stable. These solutions, known as instantons or multi-instantons, realize a mapping of the three-dimensional sphere at infinity on the gauge group, and the topological charge is the winding number of this mapping. The Jacobian of this mapping is the Chern

current K_μ and its divergence $\partial_\mu K_\mu(x) \equiv Q(x)$ is the density of topological charge. $Q = \int d^4x\, Q(x)$ is the topological charge which has integer values. Explicitly,

$$Q(x) = \frac{g^2}{16\pi^2} \mathrm{tr}[G_{\mu\nu} G^*_{\mu\nu}] \qquad [28]$$

with $G^*_{\mu\nu} = (1/2)\epsilon_{\mu\nu\rho\sigma} G_{\rho\sigma}$ the dual field strength tensor.

$Q(x)$ plays an important role in hadron physics, being related to the anomaly of the flavor singlet axial current $J^5_\mu = \sum_f \bar{\psi}\gamma^5\gamma_\mu\psi_f$. J^5_μ is conserved at the classical level in the chiral limit $m_f = 0$, but this symmetry does not survive quantization. In fact,

$$\partial_\mu J^5_\mu = 2N_f Q(x) \qquad [29]$$

A consequence of eqn [29] is the high mass $m_{\eta'} \approx 1\,\mathrm{GeV}$ of the flavor singlet partner η' of the pseudoscalar flavor octet. An $N_c \to \infty$ argument by Witten and Veneziano relates $m_{\eta'}$ to the response of the quenched (no quark) vacuum to topological excitation, the topological susceptibility $\chi \equiv \int d^4x < 0|TQ(x)Q(0)|0 >$. The relation is

$$\frac{2N_f}{f^2_\pi}\chi = [m^2_{\eta'} + m^2_\eta - 2m^2_K][1 + O(1/N_c)] \qquad [30]$$

This approximate relation has been checked on the lattice. χ has been determined by different methods which agree in confirming it. This is an important verification of QCD.

Instantons are stable solutions in the continuum, approximately stable in the lattice discretized version. A cooling procedure which locally freezes short-distance quantum fluctuations would leave the instantons untouched if they were stable. On the lattice the instanton is stable anyhow if the distance in correlation reached by the local cooling procedure is small compared to the size of the instanton: cooling is indeed a diffusion process and the distance involved grows as the square root of the number of cooling iterations. Instanton configurations can nicely be exposed by cooling.

See also: Anomalies; Quantum Chromodynamics; Renormalization: General Theory; Spin Foams; Symmetry Breaking in Field Theory.

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Leray–Schauder Theory and Mapping Degree

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Introduction

The Leray–Schauder theory gives a powerful and versatile continuation method for proving the existence, multiplicity, and bifurcation of solutions of nonlinear operator, differential and integral equations. Let X and Y be topological spaces, $A \subset X$, $f: X \to Y$, a continuous mapping, and $y \in Y$. The fundamental idea of a continuation method to solve the equation $f(x) = y$ in A consists in embedding it into a one-parameter family of equations

$$F(x, \lambda) = z(\lambda) \qquad [1]$$

where the continuous functions $F: X \times [0, 1] \to Y$, $z: [0, 1] \to Y$ are chosen in such a way that $F(\cdot, 1) = f, z(1) = y$ and

1. equation $F(x, 0) = z(0)$ has a nonempty set of solutions in A;
2. one of those solutions at least can be continued into a solution in A of [1] for each $\lambda \in [0, 1]$.

Simple examples show that Assertion 2 can be violated when all solutions of [1] leave A after some

$\lambda^* \in]0,1[$. A way to avoid such a situation consists in "closing the boundary," through the "boundary condition":

$$F(x,\lambda) \neq z(\lambda) \quad \text{for each} \quad (x,\lambda) \in \partial A \times [0,1]$$

When this condition is satisfied, Assertion 2 can still fail when two existing solutions for λ small disappear after coalescing at some $\lambda_0 < 1$. Losing all solutions through this process can be eliminated by reinforcing Assumption 1 into

2′. Equation $F(x,0) = z(0)$ has a "robust" nonempty set of solutions in A.

This statement can be made precise through the concept of topological degree of a mapping, an "algebraic" count of the number of its zeros. In a finite-dimensional setting, this concept was introduced by Kronecker for smooth mappings and by Brouwer for continuous mappings. Its extension by Leray and Schauder to some classes of mappings in Banach spaces made much wider applications to nonlinear differential and integral equations possible.

Topological Degree of a Mapping

If $U \subset \mathbb{R}^n$ is a bounded open set, $z \in \mathbb{R}^n$ and $F:\bar{U} \to \mathbb{R}^n$ is a C^1 mapping such that $z \notin F(\partial U)$ and $\det F'(x) \neq 0$ on $F^{-1}(z)$, the Brouwer degree $\deg_B[F,U,z]$ is defined (analytically) by

$$\deg_B[F,U,z] := \sum_{x\in F^{-1}(z)} \operatorname{sign} \det F'(x) = \sum_{x\in F^{-1}(z)} (-1)^{\sigma(x)}$$

where $\sigma(x)$ is the sum of the multiplicities of the negative eigenvalues of $F'(x)$. The case of a continuous F such that $z \notin F(\partial U)$ is treated by approximating F through mappings of the above type, and showing that the corresponding degrees stabilize to an unique value, defining $\deg_B[F,U,z]$ in the general case. This number remains the same under sufficiently small perturbations of F and/or z, which expresses the "robustness" mentioned above. When $n = 2$ and U is bounded by a closed Jordan curve, then $\deg_B[F,U,0]$ is nothing but the winding number of $F/\|F\|$ along ∂U.

Leray and Schauder have extended Brouwer degree to the important class of compact perturbations of identity in a normed space. A compact mapping $f:A \to B$ between metric spaces is a continuous mapping on A such that $f(A)$ is relatively compact. If $f:A \to B$ is continuous and compact on each bounded $B \subset A$, f is called "completely continuous" on A.

If X is a real normed space, $U \subset X$ an open bounded set, $f:\bar{U} \to X$ compact, and $z \notin (I-f)(\partial U)$, the Leray–Schauder degree $\deg_{LS}[I-f,U,z]$ of $I-f$ in U over z is constructed from Brouwer degree by approximating the compact mapping f over $\bar{U}$ by mappings f_ϵ with range in a finite-dimensional subspace X_ϵ of X containing z. One shows that the values of the Brouwer degrees $\deg_B[(I-f_\epsilon)|_{X_\epsilon}, U \cap X_\epsilon, z]$ stabilize for sufficiently small positive ϵ to a common value which defines $\deg_{LS}[I-f,U,z]$.

Again, this topological degree is an algebraic count of the number of elements of $(I-f)^{-1}(z)$, equal to 0 when $z \notin (I-f)(U)$. When f is of class C^1, and $I - f'(x)$ invertible at each fixed point $x \in (I-f)^{-1}(z)$, $(I-f)^{-1}(z)$ is finite and the Leray–Schauder formula holds:

$$\deg_{LS}[I-f,U,z] = \sum_{x\in(I-f)^{-1}(z)} (-1)^{\sigma(x)} \qquad [2]$$

where $\sigma(x)$ is the sum of the algebraic multiplicities of the eigenvalues of $f'(x)$ contained in $[1,+\infty]$.

Let $I = [0,1]$. For $A \subset X \times I$, and $\lambda \in I$, we write $A_\lambda = \{x \in X : (x,\lambda) \in A\}$. The Leray–Schauder degree inherits the basic properties of Brouwer degree:

1. *Additivity*. If $U = U_1 \cup U_2$, where U_1 and U_2 are open and disjoint, and if $z \notin (I-f)(\partial U_1) \cup (I-f)(\partial U_2)$, then
$$\deg_{LS}[I-f,U,z] = \deg_{LS}[I-f,U_1,z] + \deg_{LS}[I-f,U_2,z]$$
2. *Existence*. If $\deg_{LS}[I-f,U,z] \neq 0$, then $z \in (I-f)(U)$.
3. *Homotopy invariance*. Let $\Omega \subset X \times I$ be a bounded open set, and let $F:\bar{\Omega} \to X$ be compact. If $x - F(x,\lambda) \neq z$ for each $(x,\lambda) \in \partial\Omega$, then $\deg_{LS}[I - F(\cdot,\lambda), \Omega_\lambda, z]$ is independent of λ.

In particular, if a is an isolated fixed point of f, and $B(a,r)$ denotes the open ball of center a and radius r, $\deg_{LS}[I-f,B(a,r),0]$ is defined and independent of r for sufficiently small $r > 0$. Its value is called the "Leray–Schauder index" of $I-f$ at a, and denoted by $\operatorname{ind}_{LS}[I-f,a]$.

Fixed-Point Theorems for Compact Perturbations of Identity in a Normed Space

An important application of Leray–Schauder degree is the obtention of general fixed point theorems for compact mappings in normed spaces based on

continuation along a parameter. If $F: A \subset X \times I \to X$, we denote by Σ^A the (possibly empty) solution set defined by

$$\Sigma^A = \{(x, \lambda) \in A : x = F(x, \lambda)\}$$

Let $\Omega \subset X \times I$ be a bounded open set and $F: \bar{\Omega} \to X$ be a compact mapping. The general Leray–Schauder fixed-point theorem goes as follows:

Theorem *If the following conditions hold*:

(i) $\Sigma^{\bar{\Omega}} \cap \partial\Omega = \emptyset$ (*a priori estimate*)
(ii) $\deg_{LS}[I - F(\cdot, 0), \Omega_0, 0] \neq 0$ (*degree condition*), *then* $\Sigma^{\bar{\Omega}}$ *contains a continuum* $\mathcal{C}$ *along which* λ *takes all values in* I. In other words, $\Sigma^{\bar{\Omega}}$ contains a compact connected subset $\mathcal{C}$ connecting $\Sigma_0^{\bar{\Omega}}$ to Ω_1. If one refines Assumption (ii) into
(iii) $\Sigma_0^{\bar{\Omega}}$ *is a finite nonempty set* $\{a_1, \ldots, a_\mu\}$ and $\mathrm{ind}_{LS}[I - F(\cdot, 0), a_1] \neq 0$, the conclusion takes the form of an "alternative": *if assumptions* (i) *and* (iii) *hold, then* $(a_1, 0)$ *belongs either to a continuum in* $\Sigma^{\bar{\Omega}}$ *containing one of the points* $(a_2, 0), \ldots, (a_\mu, 0)$, *or to a continuum in* $\Sigma^{\bar{\Omega}}$ *along which* λ *takes all the values in* I.

Condition (iii) automatically holds in the following important special case: If $\Sigma^{\bar{\Omega}} \cap \partial\Omega = \emptyset$, $F(\cdot, 0) = 0$, and $0 \in \Omega_0$, then $\Sigma^{\bar{\Omega}}$ contains a continuum $\mathcal{C} \ni (0, 0)$ along which λ takes all values in I. When dealing with the fixed-point problem $x = f(x)$ with $f: \bar{U} \subset X \to X$ compact, U open and bounded, a natural choice is $F(x, \lambda) = \lambda f(x), \Omega = U \times I$, giving the statement: If $0 \in U$ and if $x \neq \lambda f(x)$ for each $(x, \lambda) \in \partial U \times I$, then $\{(x, \lambda) \in \bar{U} \times I : x = \lambda f(x)\}$ contains a continuum $\mathcal{C} \ni (0, 0)$ along which λ takes all values in I.

Condition (i) requires the *a priori* knowledge of the localization of the solution set $\Sigma^{\bar{\Omega}}$ and is in general very difficult to check. An important special case occurs when Σ^X is *a priori* bounded: if F is completely continuous on $X \times I$, $F(\cdot, 0) = 0$, and $\Sigma^X \subset B(r) \times I$ for some $r > 0$, then Σ^X contains a continuum $\mathcal{C} \ni (0, 0)$ along which λ takes all values in I. Its special case with $F(\lambda, x) = \lambda f(x)$ can be stated as Schaefer's alternative: Let $f: X \to X$ be completely continuous. Then either there exists, for each $\lambda \in [0, 1]$, at least one $x \in X$ such that $x = \lambda f(x)$, or the fixed point set $\{x \in X : x = \lambda f(x), 0 < \lambda < 1\}$ is unbounded in X. Schaefer's alternative is equivalent to the following Schauder fixed-point theorem:

Theorem *Any compact mapping* $f: \overline{B(r)} \to \overline{B(r)}$ *has a fixed point.*

A simple consequence of Schauder's theorem is that, for any continuous and bounded $g: \mathbb{R} \to \mathbb{R}$, any open bounded $D \subset \mathbb{R}^n$, any λ different from an eigenvalue of $-\Delta$ on D with Dirichlet boundary conditions, the nonlinear Dirichlet problem

$$\Delta u + \lambda u + g(u) = h(x) \quad \text{in } D$$
$$u = 0 \quad \text{on } \partial D$$

has a weak solution for each $h \in L^2(D)$.

An interesting consequence of Leray–Schauder theorem with Σ^X *a priori* bounded is that, for any bounded domain $D \subset \mathbb{R}^n$ with ∂D of class C^2, the Dirichlet problem for the equation of surfaces with constant mean curvature Λ

$$(1 + \|\nabla u\|^2)\Delta u - \sum_{i,j=1}^{n} \partial_i u \, \partial_j u \, \partial_{ij}^2 u = n\Lambda(1 + \|\nabla u\|^2)^{3/2}$$

has a unique solution for arbitrary smooth boundary data if and only if the mean curvature of the boundary ∂D is everywhere greater than $[n/(n-1)]|\Lambda|$.

The use of auxiliary continuous functionals gives a fixed-point theorem in the absence of *a priori* bounds:

Theorem (Capietto–Mawhin–Zanolin). *Let* $\Omega \subset X \times I$ *be an open set and* $F: \bar{\Omega} \to X$ *be completely continuous. If* $\Sigma_0^{\bar{\Omega}}$ *is bounded,* $\deg_{LS}[I - F(\cdot, 0), U_0, 0] \neq 0$ *for some open bounded neighborhood* U_0 *of* $\Sigma_0^{\bar{\Omega}}$, *and if there exists a continuous mapping* $\varphi: X \times I \to \mathbb{R}_+$, *proper on* $\Sigma^{\bar{\Omega}}$, *and* $c_- < \min_{\Sigma_0^{\bar{\Omega}}} \varphi(\cdot, 0) \leq \max_{\Sigma_0^{\bar{\Omega}}} \varphi(\cdot, 0) < c_+$ *such that* $\Sigma^{\bar{\Omega}} \notin \{c_-, c_+\}$ *and* $\Sigma^{\partial\Omega} \notin [c_-, c_+]$, *then* $\Sigma^{\bar{\Omega}}$ *contains a continuum* $\mathcal{C}$ *along which* λ *takes all values in* I.

This result implies, for example, that for $g: \mathbb{R} \to \mathbb{R}$ continuous, odd and superlinear ($\lim_{|u| \to \infty} g(u)/u = +\infty$), and $p: [0, 1] \times \mathbb{R}^2$ with at most linear growth in u and u' at infinity, the two-point boundary-value problem

$$u'' + g(u) = p(t, u, u'), \quad u(0) = u(1) = 0$$

has, for all sufficiently large j, at least one solution u_j having exactly $j + 1$ zeros on $[0, 1]$, and $\|u_j\|_{C^1} \to \infty$ if $j \to \infty$.

Extensions of Leray–Schauder degree

Fixed-point theorems for operators between suitable nonlinear spaces can also be proved using topological continuation arguments. For example, if $C \subset X$ is a nonempty convex set, one has the following extension of a result of the previous section to mappings in C: if $U \subset C$ is open and bounded, $F: \mathrm{cl}_C U \times I \to C$ compact and such that $x \neq F(x, \lambda)$ for each $(x, \lambda) \in \partial_C U \times I$, $F(\cdot, 0) = x_0 \in U$, then

$F(\cdot, \lambda)$ has a fixed point in U for each $\lambda \in I$. The special case where C is a wedge is useful in finding positive solutions of nonlinear differential or integral equations. For nonlinear spaces, the degree has to be replaced by the fixed-point index, which generalizes both the "Hopf–Lefschetz number" and Leray–Schauder degree.

The Leray–Schauder degree also has been extended to other classes of operators. Compact operators can be replaced by k-set-contractive or condensing mappings f, with respect to various measures of noncompactness, and fixed-point problems can be replaced by problems of the form $x \in F(x)$ for multivalued mappings F. Equivariant degree theories have been developed when U is invariant and f equivariant with respect to the action of some compact Lie group G on X. The special case of $G = S^1$ is of special importance in the study of periodic solutions of autonomous differential systems. Degree theories have also been constructed for various classes of mappings between two different Banach spaces or manifolds, which include monotone-like and nonlinear Fredholm operators. We just describe a simple but useful situation in this direction.

Many differential equations, when expressed as equations in an abstract space, do not have the fixed-point form but can be written as $Lx = Nx$ with $L: D(L) \subset X \to Z$ linear, $N: \bar{U} \to Z$, X and Z real normed spaces. If L is invertible, the equation is trivially equivalent to the fixed-point problem $x = L^{-1}Nx$, to which Leray–Schauder theory can be applied when $L^{-1}N$ is compact. The situation is more delicate when L has no inverse. If L is a linear Fredholm mapping of index zero (its range $R(L)$ is closed and has a finite codimension equal to the dimension of its null space $N(L)$), the set $\mathcal{F}(L)$ of linear continuous mappings of finite rank $A: X \to Z$ such that $L + A: D(L) \to Z$ is a bijection is nonempty and the compactness of $(L+A)^{-1}G$ does not depend upon the choice of $A \in \mathcal{F}(L)$. G is then called "L-compact" on E, and "L-completely continuous" on E when compact on each bounded set of E.

The following continuation theorem for perturbed Fredholm mapping of index zero holds.

Theorem *Let $\Omega \subset X \times I$ be open and bounded, $L: D(L) \subset X \to Z$ linear Fredholm of index zero, $N: \bar{\Omega} \to Z$ L-compact, and let $\Sigma = \{(x,\lambda) \in (D(L) \times I) \cap \bar{\Omega}: Lx = N(x,\lambda)\}$. If*

(i) *$\Sigma \cap \partial\Omega \neq \emptyset$ (a priori estimate),*
(ii) *$N(\bar{\Omega}_0 \times \{0\}) \subset Y$, with $Y \oplus R(L) = Z$ (transversality condition), and*
(iii) *$\deg_B[N(\cdot, 0)|_{\ker L}, \Omega_0 \cap \ker L, 0] \neq 0$ (degree condition)*

then Σ contains a continuum C along which λ takes all values in I.

When dealing with equation $Lx = f(x)$ with f L-completely continuous, an interesting special case of the above result follows from the choice $N(x,\lambda) = \lambda f(x) + (1-\lambda)Qf(x)$, with $Q: Z \to Z$ a projector such that $N(Q) = R(L)$. In this case, the homotopy is equivalent to

$$\begin{aligned} Lx &= \lambda f(x) \quad (\lambda \in]0,1]) \\ Qf(x) &= 0;\ x \in N(L) \quad (\lambda = 0) \end{aligned}$$

An application (among many) of this result, for $g: \mathbb{R} \to \mathbb{R}$ continuous such that $-\infty < \limsup_{u \to -\infty} g(u) < \liminf_{u \to +\infty} g(u) < +\infty$, $D \subset \mathbb{R}^n$ open, bounded, λ_k an eigenvalue of the Dirichlet problem for $-\Delta$ on D, is the weak solvability of the nonlinear problem

$$\begin{aligned} \Delta u + \lambda_k u + g(u) &= h(x) \quad \text{in } D \\ u &= 0 \quad \text{on } \partial D \end{aligned}$$

for each $h \in L^2(D)$ such that

$$\int_D h(x)\varphi(x)\,\mathrm{d}x < \left[\limsup_{u \to -\infty} g(u)\right] \times \int_D \varphi^+(x)\,\mathrm{d}x - \left[\liminf_{u \to +\infty} g(u)\right] \int_D \varphi^-(x)\,\mathrm{d}x$$

for all eigenfunctions φ associated to λ_k. The addition of the nonlinearity g "widens" the range $\{h \in L^2(D): \int_D h\varphi = 0\}$ of the corresponding linear problem.

Bifurcation Theory

Leray–Schauder degree is a powerful tool in bifurcation theory, where, given a family $\mathcal{F}$ of solutions, one tries to detect and analyze other ones branching or bifurcating from $\mathcal{F}$. Consider the equation

$$x = \lambda Lx + R(x, \lambda) \qquad [3]$$

in a real normed space X, where $L: X \to X$, linear, and $R: X \times \mathbb{R} \to X$ are completely continuous, and $R(0,\lambda) = 0$ for each $\lambda \in \mathbb{R}$. Thus, $\{(0,\lambda): \lambda \in \mathbb{R}\}$ is the trivial solution set of [3]. A bifurcation point $(\lambda^*, 0)$ for [3] is the limit of a sequence (λ_k, x_k) of solutions of [3] in $\mathbb{R}\setminus\{0\}$.

If

$$\lim_{x \to 0} \frac{\|R(x,\lambda)\|}{\|x\|} = 0 \quad \text{uniformly on bounded } \lambda\text{-sets} \qquad [4]$$

it is easy to prove that if $(\lambda^*, 0)$ is a bifurcation point for [3], then λ^* is a characteristic value (reciprocal of an eigenvalue) of L. Leray–Schauder theory gives a partial

converse to this result known as Krasnosel'skii's bifurcation theorem:

Theorem *For each real characteristic value λ^* of L with odd algebraic multiplicity, $(\lambda^*, 0)$ is a bifurcation point of* [3]. Of fundamental importance in the proof is the special case of [2] with $f = L$ and $N(I - L) = \{0\}$.

Another fruitful concept is Krasnosel'skii's bifurcation from infinity. We say (λ^*, ∞) is a bifurcation point for [3] if there exists a sequence (λ_n, x_n) of solutions of [3] such that $\lambda_n \to \lambda^*$ and $\|x_n\| \to \infty$. The corresponding bifurcation result goes as follows (Krasnosel'skii): if

$$\lim_{\|x\| \to \infty} \frac{\|R(x, \lambda)\|}{\|x\|} = 0 \quad \text{uniformly on bounded } \lambda\text{-sets} \qquad [5]$$

then, for each real characteristic value λ^* of L with odd algebraic multiplicity, (λ^*, ∞) is a bifurcation point of [3].

Global versions of Krasnosel'skii's theorems can be given, whose statements are reminiscent of Leray–Schauder's alternative theorem. Let $\mathcal{S}$ denote the closure in $\mathbb{R} \times X$ of the set of $(\lambda, x) \in \mathbb{R} \times (X \setminus \{0\})$ satisfying [3]. For bifurcation from zero, one has Rabinowitz global bifurcation theorem:

Theorem *If* [4] *holds and λ^* is a real characteristic value of L with odd algebraic multiplicity, then $\mathcal{S}$ contains a component $\mathcal{C}$ which either is unbounded, or contains $(\lambda^{**}, 0)$, where $\lambda^{**} \neq \lambda^*$ is a characteristic value of L.*

As an application, one can show that the nonlinear Sturm–Liouville problem

$$-(p(x)u')' + q(x)u = \lambda a(x)u + h(x, u, u', \lambda) \quad (x \in]0, 1[)$$
$$a_0 u(0) + b_0 u'(0) = a_1 u(1) + b_1 u'(1) = 0$$

with $p \in C^1$ positive, q, a, h continuous, a positive, $(a_0^2 + b_0^2)(a_1^2 + b_1^2) \neq 0$ and $h(x, u, v) = o(|u| + |v|)$ if $|u| + |v| \to 0$ uniformly on compact λ-intervals, has, for each $k \in \mathbb{N}$, an unbounded component of solution $\mathcal{C}_k$ in $\mathbb{R} \times C^1([0, 1])$ emanating from $(\lambda_k, 0)$, with λ_k an eigenvalue of the problem with $h \equiv 0$ (Rabinowitz).

One has also global bifurcation from infinity: if [5] holds and if λ^* is a real characteristic value of L with odd algebraic multiplicity, then [3] has an unbounded component of solutions $\mathcal{D}$ which contains (λ^*, ∞).

See also: Bifurcation Theory; Bifurcations in Fluid Dynamics; Bifurcations of Periodic Orbits; Minimal Submanifolds; Minimax Principle in the Calculus of Variations; Partial Differential Equations: Some Examples; Riemann–Hilbert Problem; Topological Defects and Their Homotopy Classification; Viscous Incompressible Fluids: Mathematical Theory.

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Lie Bialgebras *see* Classical *r*-Matrices, Lie Bialgebras, and Poisson Lie Groups

Lie Groups: General Theory

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Introduction

Local continuous transformations were introduced by Lie as a tool for solving ordinary differential equations. In this program, he followed the spirit of Galois, who used finite groups to develop algorithms for solving algebraic equations (the general quadratic, cubic, and quartic), or else to prove that some equations (the generic quintic) could not be solved by quadrature.

Lie's work led eventually to the definition and study of Lie groups. Lie groups are beautiful in their own right – so beautiful that they have been studied independently of their origin as a tool for solving differential equations and studying the special functions determined by certain classes of these equations.

Lie Groups

Lie groups exist at the interface of the two great divisions of mathematics: algebra and topology. Their algebraic properties derive from the group axioms. Their geometric properties arise from the parametrization of the group elements by points in a differentiable manifold. The rigidity of these structures arises from the continuity requirements imposed on the group composition and inversion maps.

The algebraic axioms are standard.

Definition A group G consists of a set $g_i, g_j, g_k, \ldots \in G$ together with a combinatorial operation $\circ$ that satisfy the four axioms:

(i) *Closure*. If $g_i \in G, g_j \in G$, then $g_i \circ g_j \in G$.
(ii) *Associativity*. If $g_i, g_j, g_k \in G$, then $(g_i \circ g_j) \circ g_k = g_i \circ (g_j \circ g_k)$.
(iii) *Identity*. There is a unique operation $e \in G$ that satisfies $e \circ g_i = g_i = g_i \circ e$.
(iv) *Inverse*. Every group operation $g_i \in G$ has an inverse, denoted g_i^{-1}, that satisfies $g_i \circ g_i^{-1} = e = g_i^{-1} \circ g_i$.

Lie groups have more structure than groups. In particular, each $g_i \in G$ is a point in an n-dimensional manifold M^n. That is, the subscript i actually identifies a point $x \in M^n$, so that we can write $g_i = g(x)$ or most simply $g_i = x$. The group multiplication can be expressed in the form $g_i \circ g_j = g_k \to g(x) \circ g(y) = g(z)$, where $x \in M^n$, $y \in M^n, z = \phi(x, y) \in M^n$. The group inversion map can be expressed in the form $g(x) \to g(x)^{-1} = g(y)$, $y = \psi(x) \in M^n$. The topological axioms for Lie groups can be taken as:

(v) *Continuity of composition*. The mapping $z = \phi(x, y)$ defined by the group composition law is differentiable.
(vi) *Continuity of inversion*. The mapping $y = \psi(x)$ defined by the group inversion law is differentiable.

The dimension of the Lie group is the dimension of the manifold that parametrizes the operations in the group.

The most familiar examples of Lie groups consist of $n \times n$ nonsingular matrices over the fields R, C, Q of real numbers, complex numbers, and quaternions. For example, the set of 2×2 real unimodular matrices

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad ad - bc = 1$$

is a three-dimensional submanifold embedded in $R^{2^2} = R^4$.

Matrix Lie Groups

Not every Lie group is a matrix group. Yet, it is a surprising and useful result that almost every Lie group encountered in physics is a matrix Lie group. These are all subgroups of the general linear groups $\mathrm{GL}(n; F)$ of $n \times n$ nonsingular matrices over the field F (R, C, Q). These groups have real dimension $n^2 \times (1, 2, 4)$, respectively. The special linear subgroups $\mathrm{SL}(n; F)$ are defined as the subgroups of $n \times n$ matrices with determinant $+1$: $M \in \mathrm{SL}(n; F)$ if $\det M = +1$. This definition is problematic for quaternions, as they do not commute. To avoid this problem, it is useful to map quaternions into 2×2 complex matrices in the same way complex numbers can be mapped into 2×2 real matrices:

$$a + \mathrm{i}b \to \begin{bmatrix} a & b \\ -b & a \end{bmatrix}$$

$$q_0 + \mathcal{I}q_1 + \mathcal{J}q_2 + \mathcal{K}q_3 \to \begin{bmatrix} q_0 + \mathrm{i}q_3 & \mathrm{i}q_1 + q_2 \\ \mathrm{i}q_1 - q_2 & q_0 - \mathrm{i}q_3 \end{bmatrix}$$

Here $(1, \mathrm{i})$ are basis vectors for C^1 considered as a real two-dimensional linear vector space,

$(1,\mathcal{I},\mathcal{J},\mathcal{K})$ are basis vectors for Q^1 considered as a real four-dimensional linear vector space, and (a,b) and (q_0,q_1,q_2,q_3) are all real. The squares of the imaginary quantities i and $\mathcal{I},\mathcal{J},\mathcal{K}$ are all -1: $\mathrm{i}^2=-1$; $\mathcal{I}^2=\mathcal{J}^2=\mathcal{K}^2=-1$ and the imaginary quaternion basis elements anticommute: $\{\mathcal{I},\mathcal{J}\}=\{\mathcal{J},\mathcal{K}\}=\{\mathcal{K},\mathcal{I}\}=0$. The unimodular subgroup $SL(n;Q)$ of $GL(n;Q)$ is obtained by replacing each quaternion matrix element by a 2×2 complex matrix, setting the determinant of the resulting $2n\times 2n$ matrix group to $+1$, and then mapping each of the n^2 complex 2×2 matrices back to quaternions.

Many other important groups are defined by imposing linear or quadratic constraints on the n^2 matrix elements of $GL(n;F)$ or $SL(n;F)$. The compact metric-preserving groups $U(n;F)$ leave invariant lengths (preserve a positive-definite metric $g=I_n$) in linear vector spaces. The matrices $M\in U(n;F)$ satisfy $M^\dagger I_n M=I_n$. These conditions define the orthogonal groups $O(n)=U(n;R)$ and the unitary groups $U(n)=U(n;C)$. Their noncompact counterparts $O(p,q)$ and $U(p,q)$ leave invariant nonsingular indefinite metrics

$$g=I_{p,q}=\begin{bmatrix} I_p & 0 \\ 0 & -I_q\end{bmatrix}$$

in real and complex $n=(p+q)$-dimensional linear vector spaces: $M^\dagger I_{p,q}M=I_{p,q}$.

Intersections of matrix Lie groups are also Lie groups. The special metric-preserving groups are intersections of the special linear groups $SL(n;F)\subset GL(n;F)$ (with $F=Q$, $SL(n;Q)$ is defined as described above) and the metric-preserving subgroups $U(n;F)\subset GL(n;F)$:

$$\begin{aligned}
&SL(n;R)\cap U(n;R)=SO(n), && n(n-1)/2\\
&SL(n;C)\cap U(n;C)=SU(n), && n^2-1\\
&SL(n;Q)\cap U(n;Q)=Sp(n)\Rrightarrow USp(2n), && n(2n+1)
\end{aligned}$$

The real dimensions of these groups are given in the right-hand column. Under the replacement of quaternions by 2×2 complex matrices, the group of $n\times n$ metric-preserving and unimodular matrices $Sp(n)$ over Q is identified as $USp(2n)$, an isomorphic group of $2n\times 2n$ matrices over C.

Noncompact forms $SO(p,q)$, $SU(p,q)$, and $Sp(p,q)=USp(2p,2q)$ are defined similarly.

The Lie group SU(2) rotates spin states to spin states in a complex two-dimensional linear vector space. It leaves lengths, inner products, and probabilities invariant. If an interaction is spin independent, only an invariant ("Casimir invariant") constructed from the spin operators can appear in the Hamiltonian. The same group can act in isospin space, rotating proton to neutron states. The Lie group SU(3) similarly rotates quark states or color states into quark states or color states, respectively. The Lie group SU(4) rotates spin–isospin states into themselves. The conformal group SO(4,2) leaves angles but not lengths in spacetime invariant. It is the largest group that leaves the source-free Maxwell equations invariant. It is also the largest group that transforms all the (bound, scattering, and parabolic) hydrogen atom states into themselves.

Lie groups such as the Poincaré group (inhomogeneous Lorentz group) and the Galilei group have the matrix structures

$$\left[\begin{array}{cccc|c} & & & & t_1\\ & O(3,1) & & & t_2\\ & & & & t_3\\ & & & & t_4\\ \hline 0 & 0 & 0 & 0 & 1\end{array}\right]\begin{bmatrix} x\\ y\\ z\\ ct\\ 1\end{bmatrix}$$

$$\left[\begin{array}{ccc|cc} & & & v_1 & t_1\\ & O(3) & & v_2 & t_2\\ & & & v_3 & t_3\\ \hline 0 & 0 & 0 & 1 & t_4\\ 0 & 0 & 0 & 0 & 1\end{array}\right]\begin{bmatrix} x\\ y\\ z\\ t\\ 1\end{bmatrix}$$

respectively. In these transformations $\boldsymbol{t}=(t_1,t_2,t_3)$ describes translations in the space (x-, y-, and z-) directions, $\boldsymbol{v}=(v_1,v_2,v_3)$ describes boosts, and t_4 resets clocks. The matrices in these defining matrix representations are reducible.

The Heisenberg covering group H_4 is a four-dimensional Lie group with a simple 3×3 matrix structure:

$$\text{Heisenberg covering group}=H_4=\begin{bmatrix} 1 & l & d\\ 0 & n & r\\ 0 & 0 & 1\end{bmatrix},\quad n\neq 0$$

This matrix representation of H_4 is faithful but nonunitary.

"Linearization" of a Lie Group

At the topological level, a Lie group is homogeneous. That is, every point in a manifold that parametrizes a Lie group looks like every other point. At the algebraic level, this is not true – the identity group operation e is singled out as an exceptional group element. At the analytic level, the group composition law $z=\phi(x,y)$ is nonlinear, and can therefore be arbitrarily complicated.

The study of Lie groups is enormously simplified by exploiting these three observations. Specifically, it is useful to "linearize" the group multiplication law in the neighborhood of the identity. The linearization leads to a local Lie group. This is a linear vector space on which there is an additional structure. Once the local Lie group properties are known in the neighborhood of the identity, they are known everywhere else in the group, since the group is homogeneous.

A Lie group is linearized in the neighborhood of the identity by expressing an operator near the identity in the form $g(\epsilon)=I+\epsilon X$, where the local Lie group operator $\epsilon X=\delta x^i X_i$, the X_i are n linearly independent vector fields on the manifold M^n, and the small coordinates δx^i measure the distance (in some rough sense) of $g(\epsilon)$ from the point that parametrizes the identity group operation $e=g(0)$. For another group operation $g(\delta Y)=I+\delta Y$ in the neighborhood of the identity, the following holds.

1. The product $g(\epsilon X)g(\delta Y)=(I+\epsilon X)(I+\delta Y)=I+(\epsilon X+\delta Y)+(\text{h.o.t})$ is in the local Lie group.
2. The commutator $g_i \circ g_j \circ g_i^{-1} \circ g_j^{-1}$ in the group leads to

$$g(\epsilon X)g(\delta Y)g(\epsilon X)^{-1}g(\delta Y)^{-1} = I+\tfrac{1}{2}\epsilon\delta(XY-YX)+\text{h.o.t} = I+\tfrac{1}{2}\epsilon\delta[X,Y]+\text{h.o.t}$$

in the local Lie group.

The first condition shows that the local Lie group is a linear vector space. The n vector fields X_i can be chosen as a set of basis vectors in this space.

The second condition shows that the commutator of two vectors in this linear vector space is also in this linear vector space. The commutator endows this linear vector space with an additional combinatorial operation ("vector multiplication") and provides it with the structure of an algebra, called a Lie algebra.

Definition A Lie algebra $\mathfrak{la}$ consists of a set of operators $X, Y, Z, \ldots$, together with the operations of vector addition, scalar multiplication, and commutation $[X,Y]$ that satisfy the following three axioms:

(i) *Closure* (*linear vector space*). If $X, Y \in \mathfrak{la}$, $\alpha X+\beta Y \in \mathfrak{la}$ and $[X,Y]\in \mathfrak{la}$.
(ii) *Antisymmetry.* $[X,Y]=-[Y,X]$.
(iii) *Jacobi identity.* $[X,[Y,Z]]+[Y,[Z,X]]+[Z,[X,Y]]=0$.

The structure of a Lie algebra, or local Lie group, is summarized by the structure constants, defined in terms of the basis vectors X_i, by

$$[X_i, X_j]=c_{ij}{}^k X_k \quad \text{summation convention}$$

The structure constants $c_{ij}{}^k$ are components of a third-order tensor, covariant and antisymmetric in two indices $(c_{ij}{}^k=-c_{ji}{}^k)$ and contravariant in the third. These components obey the Jacobi identity, which places a quadratic constraint on them:

$$c_{ij}{}^s c_{sk}{}^t + c_{jk}{}^s c_{si}{}^t + c_{ki}{}^s c_{sj}{}^t = 0$$

Linearization of a Lie group generates a Lie algebra. A Lie group can be recovered by the inverse process. This is the exponential operation. A group operation a finite distance from the origin (the point identified with the identity group operation) of the manifold that parametrizes the Lie group can be obtained from the limiting procedure $(\epsilon=1/K\to 0)$:

$$g(X)=\lim_{K\to\infty}\prod\left(I+\frac{1}{K}X\right)^K = e^X = \text{EXP}(X)$$

The exponential operation is well defined for real numbers, complex numbers, quaternions, $n\times n$ matrices over these fields, and vector fields.

A 1:1 correspondence between Lie groups and Lie algebras does not exist. Isomorphic Lie groups have isomorphic Lie algebras. But nonisomorphic Lie groups may also possess isomorphic Lie algebras. The best known examples of nonisomorphic Lie groups and their isomorphic Lie algebras are

$$\begin{aligned} &SO(3)\neq SU(2), && \mathfrak{so}(3)=\mathfrak{su}(2)\\ &SO(4)\neq SU(2)\times SU(2), && \mathfrak{so}(4)=\mathfrak{su}(2)+\mathfrak{su}(2)\\ &SO(5)\neq Sp(2)=USp(4), && \mathfrak{so}(5)=\mathfrak{sp}(2)=\mathfrak{usp}(4)\end{aligned}$$

There is a 1:1 correspondence between Lie algebras and "locally" isomorphic Lie groups. This has been extended to global Lie groups by a beautiful theorem due to E Cartan.

Theorem (Cartan) *There is a 1:1 correspondence between Lie algebras and simply connected Lie groups. Every Lie group with the same Lie algebra is either the simply connected ("universal covering") group or is the quotient of this universal covering group by one of its discrete invariant subgroups.*

This relation is summarized in **Figure 1**.

As a concrete example, the Lie algebra of SO(3), which is the group of real 3×3 matrices satisfying $M^{\dagger}I_3M=I_3$ and $\det(M)=+1$, is spanned by the three "angular momentum vector

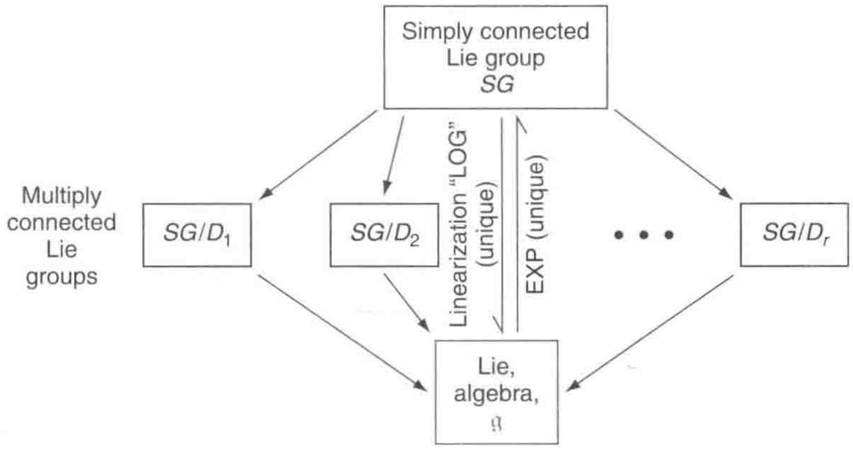


Figure 1 Cartan's theorem states that there is a 1:1 correspondence between Lie algebras and simply connected Lie groups. All other Lie groups with this Lie algebra are quotients of the covering group by one of its discrete invariant subgroups $D_j \subseteq D_{\mathrm{Max}}$. There is a relation between the discrete invariant subgroup D_j and the homotopy group of SG/D_j. Reproduced with permission from Gilmore R (1974) *Lie Groups, Lie Algebras, and Some of Their Applications*. New York: Wiley.

fields" $L_i(x) = \epsilon_{ijk}x^j\partial_k$ or the three angular momentum matrices

$$L_1 = L_{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & +1 \\ 0 & -1 & 0 \end{bmatrix}$$

$$L_2 = L_{31} = -L_{13} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ +1 & 0 & 0 \end{bmatrix}$$

$$L_3 = L_{12} = \begin{bmatrix} 0 & +1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The Lie group SU(2) is the group of complex 2×2 matrices satisfying $M^{\dagger}I_2M = I_2$ and $\det(M) = +1$. Its Lie algebra is spanned by the three spin matrices $S_j = (\mathrm{i}/2)\sigma_j$, which are multiples of the Pauli spin matrices σ_j:

$$S_1 = \frac{\mathrm{i}}{2}\begin{bmatrix} 0 & +1 \\ +1 & 0 \end{bmatrix}, \quad S_2 = \frac{\mathrm{i}}{2}\begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}$$

$$S_3 = \frac{\mathrm{i}}{2}\begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}$$

The two Lie algebras are isomorphic as they share isomorphic commutation relations $[J_1, J_2] = -J_3$ (and cyclic), $J_j = L_j$ or $J_j = S_j$. The group SU(2) is simply connected. Its maximal discrete invariant subgroup D consists of all multiples of the identity, αI_2, so that $\alpha = \pm 1$. According to Cartan's theorem, $\mathrm{SO}(3) = \mathrm{SU}(2)/D_2, D_2 = \{I_2, -I_2\}$. The group SO(3) is doubly connected, with a two-element homotopy group.

Matrix Lie Algebras

A deep theorem of Ado guarantees that every Lie algebra is equivalent to a matrix Lie algebra, even though the same is not true of Lie groups.

Sets of $n \times n$ matrices that close under vector addition, scalar multiplication, and commutation ($M_1 \in \mathfrak{a}, M_2 \in \mathfrak{a} \Rightarrow [M_1, M_2] = M_1M_2 - M_2M_1 \in \mathfrak{a}$) form matrix Lie algebras. The antisymmetry properties and Jacobi identity are guaranteed by matrix multiplication.

Lie algebras for the general linear groups $\mathrm{GL}(n; F)$ consist of $n \times n$ matrices over F. Lie algebras for the special linear groups $\mathrm{SL}(n; F)$ consist of traceless $n \times n$ matrices. The Lie algebras of the unitary groups consist of anti-Hermitian matrices. The Lie algebras of $\mathrm{U}(p, q; F)$ consist of matrices that obey

$$M^{\dagger}I_{p,q} + I_{p,q}M = 0, \quad M \in \mathfrak{u}(p, q; F)$$

The matrix Lie algebras of other matrix Lie groups are obtained by constructing the most general Lie group operation in the neighborhood of the identity by linearization. For example, the Lie algebra of the Heisenberg covering group H_4 is

$$\begin{bmatrix} 1 & l & d \\ 0 & n & r \\ 0 & 0 & 1 \end{bmatrix} \to \begin{bmatrix} 1 & \delta l & \delta d \\ 0 & 1 + \delta n & \delta r \\ 0 & 0 & 1 \end{bmatrix}$$

$$\to I_3 + \delta n\, N + \delta r\, R + \delta l\, L + \delta d\, D$$

$$N \simeq a^{\dagger}a \qquad R \simeq a^{\dagger}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$L \simeq a \qquad D \simeq I = [a, a^\dagger]$$

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The four 3×3 matrices N, R, L, D that span the Lie algebra $\mathfrak{h}_4$ of H_4 satisfy commutation relations isomorphic with the commutation relations satisfied by the photon operators ($a^\dagger a$, $a^\dagger$, a, $I = [a, a^\dagger]$). The 3×3 matrix representations of the group H_4 and the algebra $\mathfrak{h}_4$ are faithful. The representation of H_4 is nonunitary and that of $\mathfrak{h}_4$ is non-Hermitian.

There is a simple way to relate a large class of operator Lie algebras to matrix Lie algebras. If $A, B, C, \ldots$ belong to a Lie algebra of $n \times n$ matrices with $[A, B] = C$, the matrix-to-operator mapping

$$A \to \mathcal{A} = x^i A_i{}^j \partial_j$$

preserves commutation relations, for

$$\begin{aligned} [\mathcal{A}, \mathcal{B}] &= \left[x^i A_i{}^j \partial_j, x^r B_r{}^s \partial_s\right] \\ &= x^i A_i{}^j \left[\partial_j, x^r\right] B_r{}^s \partial_s - x^r B_r{}^s \left[\partial_s, x^i\right] A_i{}^j \partial_j \\ &= x^i A_i{}^j B_j{}^s \partial_s - x^r B_r{}^i A_i{}^j \partial_j = x^i [A, B]_i{}^j \partial_j = \mathcal{C} \end{aligned}$$

This relation depends on the bilinear products $x^i \partial_j$ satisfying commutation relations

$$\left[x^i \partial_j, x^r \partial_s\right] = x^i \partial_s \delta_j{}^r - x^r \partial_j \delta_s{}^i$$

These commutation relations are satisfied by products of creation and annihilation operators $a_i^\dagger a_j$ for either bosons ($b_i^\dagger b_j$) or fermions ($f_i^\dagger f_j$). These matrix-to-operator mappings can be extended to include bilinear products such as $x^i x^j$, $x^i \partial_j$, $\partial_i \partial_j$ and their boson and fermion counterparts $a_i a_j$, $a_i^\dagger a_j$, $a_i^\dagger a_j^\dagger$. For example, the vector fields associated with the operator J_1 for SO(3) and SU(2) are $x^i (L_1)_i{}^j \partial_j = x^2 \partial_3 - x^3 \partial_2$ and $u^i (S_1)_i{}^j \partial_j = (i/2)(u^1 \partial_2 + u^2 \partial_1)$.

Boson and fermion bilinear products $a_i^\dagger a_j (1 \leq i, j \leq n)$ are isomorphic to $\mathfrak{u}(n)$. Boson bilinear products $b_i b_j$, $b_i^\dagger b_j$, $b_i^\dagger b_j^\dagger$ are isomorphic to $\mathfrak{usp}(2n)$ while fermion bilinear products $f_i f_j, f_i^\dagger f_j, f_i^\dagger f_j^\dagger$ are isomorphic to $\mathfrak{so}(2n)$.

Structure of Lie Algebras

The study of Lie algebras is greatly facilitated by studying their structure. The structure is determined by the commutation properties of the Lie algebra.

Invariant Subalgebra

If a Lie algebra has an invariant subalgebra, then the commutator of anything in the algebra with anything in the subalgebra is in the subalgebra. Suppose $\mathfrak{a}$ is a linear vector subspace of $\mathfrak{g}$. If $[\mathfrak{g}, \mathfrak{a}] \subseteq \mathfrak{a}$, then $\mathfrak{a}$ is an invariant subspace of $\mathfrak{g}$. In particular, $[\mathfrak{a}, \mathfrak{a}] \subseteq \mathfrak{a}$ and $\mathfrak{a}$ is therefore also a subalgebra of $\mathfrak{g}$: it is an invariant subalgebra in $\mathfrak{g}$.

Example The Lie algebra $\mathfrak{iso}(3)$ consists of the three rotation operators $L_{ij} = x^i \partial_j - x^j \partial_i$ and the three displacement operators $P_k = \partial_k$. The subset of displacement operators is an invariant subspace in $\mathfrak{iso}(3)$, since it is mapped into itself by all commutators. It is also a subalgebra in $\mathfrak{iso}(3)$. This particular invariant subalgebra is commutative.

Solvable Algebra

If $\mathfrak{g}$ is a Lie algebra, the linear vector space obtained by taking all possible commutators of the operators in $\mathfrak{g}$ is called the "derived" algebra: $[\mathfrak{g}, \mathfrak{g}] = \mathfrak{g}^{(1)} \subseteq \mathfrak{g}$. If $\mathfrak{g}^{(1)} = \mathfrak{g}$, there is no point in continuing this process. If $\mathfrak{g}^{(1)} \subset \mathfrak{g}$, it is useful to define $\mathfrak{g} = \mathfrak{g}^{(0)}$ and to continue this process by defining $\mathfrak{g}^{(2)}$ as the derived algebra of $\mathfrak{g}^{(1)}$: $\mathfrak{g}^{(2)} = [\mathfrak{g}^{(1)}, \mathfrak{g}^{(1)}]$. We can continue in this way, defining $\mathfrak{g}^{(n+1)}$ as the algebra derived from $\mathfrak{g}^{(n)}$. Ultimately (for finite-dimensional Lie algebras), either $\mathfrak{g}^{(n+1)} = 0$ or $\mathfrak{g}^{(n+1)} = \mathfrak{g}^{(n)}$ for some n. If the former case occurs,

$$\mathfrak{g} = \mathfrak{g}^{(0)} \supset \mathfrak{g}^{(1)} \supset \mathfrak{g}^{(2)} \supset \cdots \supset \mathfrak{g}^{(n)} \supset \mathfrak{g}^{(n+1)} = 0$$

the Lie algebra $\mathfrak{g}^{(0)}$ is called solvable. Each algebra $\mathfrak{g}^{(i)}$ is an invariant subalgebra of $\mathfrak{g}^{(j)}$, $i > j$.

Example The Lie algebra spanned by the boson number, creation, annihilation, and identity operators is solvable. The series of derived algebras has dimensions 4, 3, 1, 0.

$\mathfrak{g}^{(0)}$	$\mathfrak{g}^{(1)}$	$\mathfrak{g}^{(2)}$	$\mathfrak{g}^{(3)}$
$a^\dagger a$	–	–	–
$a^\dagger$	$a^\dagger$	–	–
a	a	–	–
I	I	I	–

Semidirect Sum Algebra

When a Lie algebra $\mathfrak{g}$ has an invariant subalgebra $\mathfrak{a}$, the linear vector space of the Lie algebra $\mathfrak{g}$ can be written as the direct sum of the linear vector subspace of the subalgebra $\mathfrak{a}$ plus a complementary subspace $\boldsymbol{b}$. The subspace $\boldsymbol{b}$ is generally not by itself a Lie algebra. The Lie algebra $\mathfrak{g}$ is written as a semidirect sum of the two subspaces. The semidirect

sum structure satisfies the commutation relations shown:

$$\mathfrak{g} = \boldsymbol{b} \wedge \mathfrak{a} \qquad \begin{array}{l} [\boldsymbol{b}, \boldsymbol{b}] \subseteq \boldsymbol{b} \wedge \mathfrak{a} \\ [\boldsymbol{b}, \mathfrak{a}] \subseteq \mathfrak{a} \\ [\mathfrak{a}, \mathfrak{a}] \subseteq \mathfrak{a} \end{array}$$

The subspace $\boldsymbol{b}$ can be given the structure of an algebra modulo the component of the commutator in $\mathfrak{a}$: $\mathfrak{b} = \mathfrak{g} \bmod \mathfrak{a}$.

Example The three-dimensional Lie algebra spanned by the photon operators $a^{\dagger}$, a, I has a semidirect sum decomposition where $\boldsymbol{b}$ is spanned by $a^{\dagger}$, a and $\mathfrak{a}$ is spanned by I. The subspace $\boldsymbol{b}$ is not closed under commutation, and $\mathfrak{a}$ is commutative. The Lie algebra $\mathfrak{iso}(3)$ also has the structure of a semidirect sum, with $\boldsymbol{b} = \mathfrak{b} = \mathfrak{so}(3)$ and the invariant subalgebra $\mathfrak{a}$ is spanned by the three displacement operators P_k.

Nonsemisimple Algebra

A Lie algebra is nonsemisimple if it has a solvable invariant subalgebra.

Example The Lie algebra spanned by bilinear products of photon creation and annihilation operators $a_i^{\dagger} a_j$, creation operators $a_i^{\dagger}$, annihilation operators a_j, and the identity operator $I (1 \leq i, j \leq n)$ is nonsemisimple. The solvable invariant subalgebra is spanned by the $2n + 2$ operators consisting of the single photon operators $a_i^{\dagger}, a_j$, the identity operator I, and the total number operator $\hat{n} = \sum_{i=1}^{n} a_i^{\dagger} a_i$.

Semisimple Algebra

A Lie algebra is semisimple if it has no solvable invariant subalgebras.

Example The Lie algebra $\mathfrak{so}(4)$ is semisimple. This Lie algebra has two invariant subalgebras, both isomorphic to $\mathfrak{so}(3)$. The direct sum decomposition

$$\mathfrak{so}(4) = \mathfrak{so}(3) + \mathfrak{so}(3)$$

is well known to physical chemists and is responsible for the dualities that exist between rotating and laboratory frame descriptions of molecular systems.

Simple Algebra

A Lie algebra is simple if it has no invariant subalgebras at all. The prettiest page in the theory of Lie groups is the classification theory of the simple Lie algebras. We turn to this subject now.

Lie Algebra Tools

Two powerful tools have been developed for studying the structure of a Lie algebra. These are the regular representation and the Cartan–Killing form.

Regular Representation

This representation assigns the structure constants to a set of n $n \times n$ matrices according to

$$X_{\alpha} \to R(X_{\alpha})_{\mu}{}^{\nu} = c_{\alpha\mu}{}^{\nu}, \qquad [X_{\alpha}, X_{\mu}] = c_{\alpha\mu}{}^{\nu} X_{\nu}$$

The matrices of the regular representation contain exactly as much information as the components of the structure tensor. They can be studied by standard linear algebra methods. For example, a secular equation can be used to put the commutation relations into canonical form.

The structure of the matrices of the regular representation determines the structure of the Lie algebra. The identification is carried out according to the usual rules of representation theory, as shown in **Figure 2**. If a basis X_{α} can be found in which all the matrices of the regular representation are simultaneously reducible, the algebra possesses an invariant subalgebra. If the representation is not fully reducible, the invariant subalgebra is solvable. If the regular representation is fully reducible, the algebra consists of the direct sum of two (or more) smaller, mutually commuting subalgebras. If the regular representation is irreducible, the algebra is simple.

If a Lie algebra is solvable ($\mathfrak{solv}$), all matrices in the regular representation can be transformed to upper triangular matrices. If the Lie algebra is nilpotent ($\mathfrak{nil} \subset \mathfrak{solv}$), the diagonal matrix elements in the upper triangular matrices are zero. The converses are also true.

Cartan–Killing Form

The Cartan–Killing form is a second-order symmetric tensor that is constructed from the third-order antisymmetric tensor $c_{\alpha\mu}{}^{\nu}$ by cross-contraction

$$g_{\alpha\beta} = c_{\alpha\mu}{}^{\nu} c_{\beta\nu}{}^{\mu} = g_{\beta\alpha} = \operatorname{tr} R(X_{\alpha}) R(X_{\beta}) = (X_{\alpha}, X_{\beta}) = (X_{\beta}, X_{\alpha})$$

The metric $g_{\alpha\beta}$ can be used to place an inner product (X_{α}, X_{β}) on this linear vector space. This inner product is not necessarily positive definite.

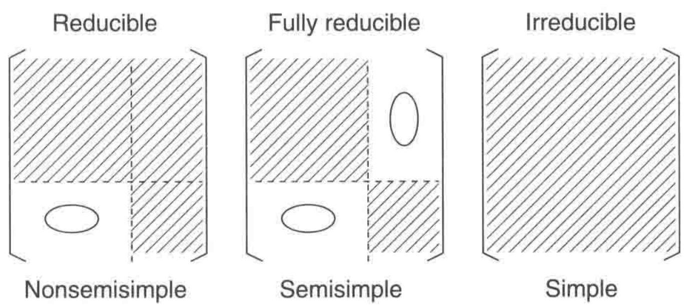


Figure 2 When the regular matrix representation of a Lie algebra is reducible, fully reducible, or irreducible, the Lie algebra is nonsemisimple, semisimple, or simple.

The matrix $g_{\alpha\beta}$ can also be treated by standard linear algebra methods. Since it is real and symmetric, it can be diagonalized. If there are n_- negative eigenvalues, n_+ positive eigenvalues, and n_0 vanishing eigenvalues ($n = n_- + n_+ + n_0$), the Lie algebra has a corresponding linear vector space decomposition of the form

$$\mathfrak{g} = \mathfrak{g}_- + \mathfrak{g}_+ + \mathfrak{g}_0$$

The inner product is positive definite on the subspace $\mathfrak{g}_+$ and negative definite on $\mathfrak{g}_-$. We call $\mathfrak{g}_0$ the singular subspace. The subspace $\mathfrak{g}_0$ is closed under commutation and in fact is a nilpotent invariant subalgebra of $\mathfrak{g}$.

Decomposition of Lie Algebras

The most general Lie algebra $\mathfrak{g}$ is the semidirect sum of a semisimple Lie algebra $\mathfrak{ss}$ and a solvable invariant subalgebra $\mathfrak{solv}$:

$$\mathfrak{g} = \mathfrak{ss} \wedge \mathfrak{solv} \qquad \begin{array}{c} [\mathfrak{ss}, \mathfrak{ss}] = \mathfrak{ss} \\ [\mathfrak{ss}, \mathfrak{solv}] \subseteq \mathfrak{solv} \\ [\mathfrak{solv}, \mathfrak{solv}] \subset \mathfrak{solv} \end{array}$$

The decomposition of $\mathfrak{g}$ into its component parts is accomplished by a simple two-step algorithm.

1. Compute the Cartan–Killing metric for $\mathfrak{g}$ and determine the singular subspace. If there is none, stop. If the dimension of $\mathfrak{g}_0 > 0$, $\mathfrak{nil} = \mathfrak{g}_0$ is the maximal nilpotent invariant subalgebra of $\mathfrak{g}$.
2. Compute the structure constants of the Lie algebra $\mathfrak{g}' = \mathfrak{g} - \mathfrak{nil} = \mathfrak{g} \bmod \mathfrak{nil} = \mathfrak{g}/\mathfrak{nil}$, the Cartan–Killing metric tensor on $\mathfrak{g}'$, and the decomposition $\mathfrak{g}' = \mathfrak{g}'_- + \mathfrak{g}'_+ + \mathfrak{g}'_0$. Then $\mathfrak{a} = \mathfrak{g}'_0$ is abelian and invariant in $\mathfrak{g}'$. In fact, $\mathfrak{a}$ is the largest abelian invariant subalgebra in $\mathfrak{g}'$.

The algorithm stops here, for the algebra $\mathfrak{g}'' = \mathfrak{g}' \bmod \mathfrak{a} = \mathfrak{g}'/\mathfrak{a} = \mathfrak{g}'_- + \mathfrak{g}'_+$ has no singular subspace under its Cartan–Killing metric.

Under this algorithm, the decomposition of $\mathfrak{g}$ into its semisimple part and its maximal solvable invariant subalgebra is

$$\mathfrak{g} = (\mathfrak{g}'_- + \mathfrak{g}'_+) \wedge (\mathfrak{g}'_0 \wedge \mathfrak{g}_0)$$

The maximum solvable invariant subalgebra $\mathfrak{solv}$ in $\mathfrak{g}$ is the semidirect sum of $\mathfrak{a}$ and $\mathfrak{nil}$: $\mathfrak{solv} = \mathfrak{g}'_0 \wedge \mathfrak{g}_0 = \mathfrak{a} \wedge \mathfrak{nil}$. In addition, $\mathfrak{ss} = \mathfrak{g} \bmod \mathfrak{solv} = \mathfrak{g}/\mathfrak{solv} = \mathfrak{g}'_- + \mathfrak{g}'_+$. The subspace $\mathfrak{g}'_-$ is closed under commutation and exponentiates into a compact subgroup of G'. The subspace $\mathfrak{g}'_+$ exponentiates to a noncompact coset in G' that is simply connected.

Every element in a semisimple Lie algebra can be expressed as the commutator of two elements in the Lie algebra. In this sense, a semisimple algebra reproduces itself under commutation.

To illustrate this algorithm, we tear apart the eight-dimensional Lie algebra spanned by the photon operators $a_i^\dagger a_j, 1 \le i, j \le 2$ and $a_3^\dagger a_3$, $a_3^\dagger$, a_3, I, where the photon operators obey $[a_i, a_j^\dagger] = \delta_{ij} I$. The regular representative of the general linear combination $X = \sum_{ij} m_{ij} a_i^\dagger a_j + n a_3^\dagger a_3 + r a_3^\dagger + l a_3 + \delta I$ is

$$R(X) = \left[\begin{array}{cccc|cccc} 0 & & -m_{12} & m_{21} & & & & \\ & 0 & m_{12} & -m_{21} & & & & \\ -m_{21} & m_{21} & +m_{11} - m_{22} & 0 & & & & \\ m_{12} & -m_{12} & 0 & -m_{11} + m_{22} & & & & \\ & & & & 0 & & & \\ & & & & & n & & l \\ & & & & & & -n & -r \\ & & & & & & & 0 \end{array}\right] \begin{array}{c} a_1^\dagger a_1 \\ a_2^\dagger a_2 \\ a_1^\dagger a_2 \\ a_2^\dagger a_1 \\ a_3^\dagger a_3 \\ a_3^\dagger \\ a_3 \\ I \end{array}$$

The Cartan–Killing inner product is the trace of the square of this matrix:

$$(X, X) = \operatorname{tr} R(X)^2 = 2(m_{11} - m_{22})^2 + 8m_{12}m_{21} + 2n^2$$

The subspace $\mathfrak{g}_0$ is spanned by $a_1^\dagger a_1 + a_2^\dagger a_2$, $a_3^\dagger$, a_3, I, leaving the four operators $a_1^\dagger a_1 - a_2^\dagger a_2, a_1^\dagger a_2$, $a_2^\dagger a_1$, $a_3^\dagger a_3$ to span $\mathfrak{g}'$. A simple calculation shows that $\mathfrak{g}'_0$ is spanned by $a_3^\dagger a_3$. As a result:

Subspace	*Spanned by*
$\mathfrak{g}'_+$	$a_1^\dagger a_1 - a_2^\dagger a_2$, $\frac{1}{\sqrt{2}}(a_1^\dagger a_2 + a_2^\dagger a_1)$
$\mathfrak{g}'_-$	$\frac{1}{\sqrt{2}}(a_1^\dagger a_2 - a_2^\dagger a_1)$
$\mathfrak{g}'_0$	$a_3^\dagger a_3$
$\mathfrak{g}_0$	$a_1^\dagger a_1 + a_2^\dagger a_2, a_3^\dagger, a_3, I$

The Lie algebra is the direct sum $\mathfrak{g} = \mathfrak{sl}(2; R) + \mathfrak{u}(1) + \mathfrak{h}_4$.

Structure of Semisimple Lie Algebras

The Cartan–Killing metric $g_{\alpha\beta}$ is nonsingular on a semisimple Lie algebra. The metric and its inverse $g^{\alpha\beta}$, can be used to raise and lower indices. In particular, the tensor whose components are $c_{\alpha\beta\gamma} = c^{\mu}_{\alpha\beta} g_{\mu\gamma}$ is third-order antisymmetric: $c_{\alpha\beta\gamma} = c_{\beta\gamma\alpha} = c_{\gamma\alpha\beta} = -c_{\beta\alpha\gamma} \ldots$. Classification of semisimple Lie algebras is equivalent to classifying such tensors.

Another useful way to describe semisimple Lie algebras is to search for a canonical structure for the commutation relations. A useful canonical form is an eigenvalue form

$$[X, Y] = \lambda Y$$

In a basis X_i, with $X = x^i X_i$ and $Y = y^j X_j$, this equation reduces to a standard eigenvalue equation for the regular representation

$$\sum_j \sum_k y^j \left(R(x^i X_i)_j{}^k - \lambda \delta_j{}^k \right) X_k = 0$$

Thus, the search for a standard form for the commutation relations reduces to a study of the secular equation

$$\det(R(X) - \lambda I) = \sum_{j=0}^{n} (-\lambda)^{n-j} \phi_j(X) = 0 \qquad [1]$$

The coefficients $\phi_j(X)$ are homogeneous polynomials of degree j in the coefficients x^i of $X = x^i X_i$.

In order to extract maximum information from this secular equation, a generic vector $X \in \mathfrak{g}$ is chosen. Such a choice minimizes all degeneracies. With a generic choice of $X \in \mathfrak{g}$, it is useful to define the rank, l, of the Lie algebra $\mathfrak{g}$ as:

1. the number of functionally independent coefficients $\phi_j(X)$ in the secular equation;
2. the number of independent roots, $\alpha_1, \alpha_2, \ldots, \alpha_l$ of the secular equation;
3. the dimension of the subspace $H \subset \mathfrak{g}$ that commutes with X; and
4. the number of independent (Casimir) operators that commute with all $X_i : \mathcal{C}_j(X) = \phi_j(x^i \to X_i)$: $[\mathcal{C}_j(X), X_i] = 0$.

For example, for $\mathfrak{so}(3)$ or $\mathfrak{su}(2)$, the secular equation for $X = x^i X_i$ is

$$\det \left[\begin{bmatrix} 0 & x_3 & -x_2 \\ -x_3 & 0 & x_1 \\ x_2 & -x_1 & 0 \end{bmatrix} - \lambda I_3 \right]$$
$$= (-\lambda)^3 + (-\lambda)\phi_2(x) = 0$$

where $\phi_2(x) = x_1^2 + x_2^2 + x_3^2$. The rank is $l = 1$. There is one independent coefficient $\phi_2(x)$ and one independent root of this equation, $\alpha_1 = \sqrt{-\delta_{ij} x^i x^j} = \mathrm{i}\sqrt{x \cdot x}$. The only linear operators that commute with X are scalar multiples of X. There is one independent homogeneous operator that commutes with all generators X_i, obtained by the substitutions $x^i \to L_i$ (for $\mathfrak{so}(3)$) or $x^i \to S_i$ (for $\mathfrak{su}(2)$):

$$\mathcal{C}^2(L) = \phi_2(x_i \to L_i) = L_1^2 + L_2^2 + L_3^2$$

The secular equation [1] is over the field of real numbers. This is not an algebraically closed field. There is no guarantee that the number of independent functions $\phi_j(x)$ in the secular equation is equal to the number of (real) roots of this equation until we extend the field from R to C, which is algebraically closed. As a result, the classification of semisimple Lie algebras is done over complex numbers. After the complex extensions of the simple Lie algebras have been classified, their different inequivalent real forms can be determined.

Root Spaces

When the secular equation for the regular representation of a generic element in a Lie algebra is solved, the commutation relations can be put into a simple and elegant canonical form. This canonical form depends on the rank, l, of the Lie algebra, not the dimension, n, of the Lie algebra. This provides a very useful simplification, as $n \sim l^2$.

For this canonical form, the independent roots $\alpha_1(x), \alpha_2(x), \ldots, \alpha_l(x)$ are gathered into a single vector $\boldsymbol{\alpha}$ with l components. The vectors $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_l)$ are called root vectors. The root vectors exist in an l-dimensional space on which a positive-definite inner product can be defined. The root vectors for a rank-l semisimple Lie algebra $\mathfrak{g}$ span this Euclidean space. The basis vectors of $\mathfrak{g}$ can be identified with the roots in the root space.

The roots in a root space have the following properties:

1. A positive-definite metric can be placed on the root space.
2. The vector 0 is a root.
3. The root 0 is l-fold degenerate.
4. If $\boldsymbol{\alpha}$ is a root and $c\boldsymbol{\alpha}$ is a root, $c = \pm 1, 0$.
5. If $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are roots,
$$\boldsymbol{\beta}' = \boldsymbol{\beta} - \frac{2\boldsymbol{\alpha} \cdot \boldsymbol{\beta}}{\boldsymbol{\alpha} \cdot \boldsymbol{\alpha}} \boldsymbol{\alpha}$$
is also a root and $2\boldsymbol{\alpha} \cdot \boldsymbol{\beta} / \boldsymbol{\alpha} \cdot \boldsymbol{\alpha}$ is an integer, n_1. In fact, $\boldsymbol{\beta}'$ is the root obtained by reflecting $\boldsymbol{\beta}$ in the hyperplane orthogonal to $\boldsymbol{\alpha}$.
6. The set of reflections generated by nonzero roots itself forms a group, the Weyl group of the Lie algebra.

7. The angle between roots $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is determined by

$$\cos^2(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{\boldsymbol{\alpha}\cdot\boldsymbol{\beta}}{\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}}\frac{\boldsymbol{\alpha}\cdot\boldsymbol{\beta}}{\boldsymbol{\beta}\cdot\boldsymbol{\beta}} = \frac{n_1}{2}\frac{n_2}{2} = 0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1$$

   The integers n_1, n_2 for noncolinear roots are constrained by $|n_1 n_2| < 4$.
8. The relative lengths of the roots are determined by the angles between them:

$\cos^2(\theta(\boldsymbol{\alpha},\boldsymbol{\beta}))$	$\theta(\boldsymbol{\alpha},\boldsymbol{\beta})$	$\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}/\boldsymbol{\beta}\cdot\boldsymbol{\beta}$
3/4	30°, 150°	$3^{\pm 1}$
2/4	45°, 135°	$2^{\pm 1}$
1/4	60°, 120°	1

9. When the roots are normalized so that

$$\sum_{\alpha\neq 0} \alpha_i \alpha_j = \delta_{ij} \quad \text{or} \quad \sum_{\alpha\neq 0} \boldsymbol{\alpha}\cdot\boldsymbol{\alpha} = l$$

   the commutation relations can be placed in the canonical form presented in the next section.

It is possible to build up all possible root space diagrams using an "Aufbau" construction. We start with a rank-1 root space. This consists of three roots in R^1: $\boldsymbol{\alpha}, 0, -\boldsymbol{\alpha}$.

To construct rank-2 root spaces, a new noncolinear root $\boldsymbol{\beta}$ is adjoined to the two nonzero roots. The new root and the old roots span R^2. The new root can only have a limited set of angles with the roots already present. The set of roots $\boldsymbol{\alpha}, \boldsymbol{\beta}$ is completed by reflection in hyperplanes orthogonal to all roots present. If any pair of roots violates the angle conditions, the result is not a root space. In this way, the rank-2 root spaces $G_2(30°), B_2 = C_2(45°), A_2(60°)$, and $D_2 = A_1 + A_1(90°)$ are constructed from A_1. Proceeding in this way, it is possible to construct rank-3 root spaces $(B_3, C_3, A_3 = D_3)$ from the rank-2 root spaces, the rank-4 root spaces from the rank-3 root spaces, and so forth. Ultimately, there are four unending chains A_n, B_n, C_n, D_n and five exceptional root spaces G_2, F_4, E_6, E_7, E_8. The rank-2 root spaces are shown in **Figure 3** and the rank-3 root spaces are shown in

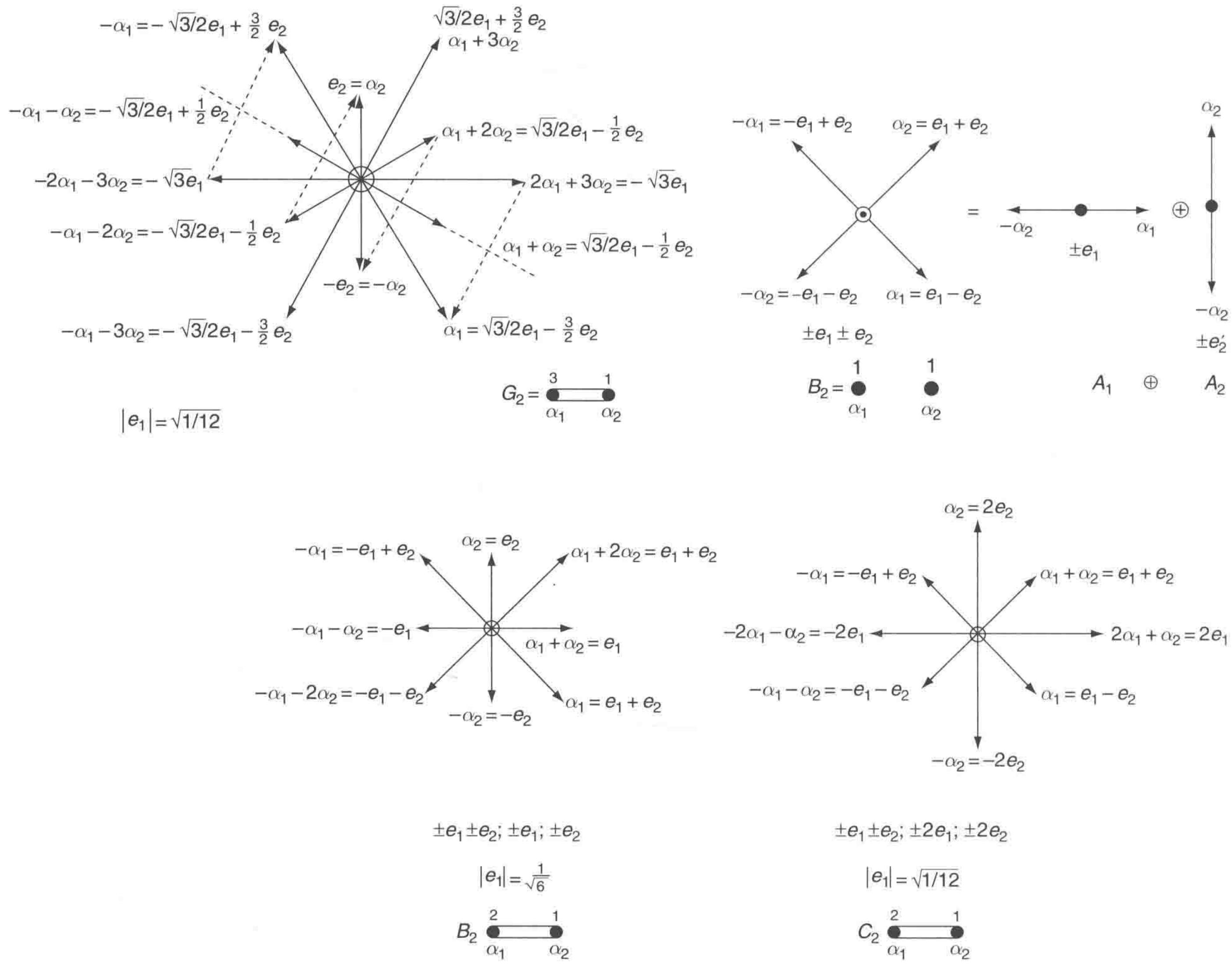


Figure 3 Rank-2 root spaces: G_2 30°, $B_2 = C_2$ 45°, A_2 60°, $D_2 = A_1 + A_1$ 90°.

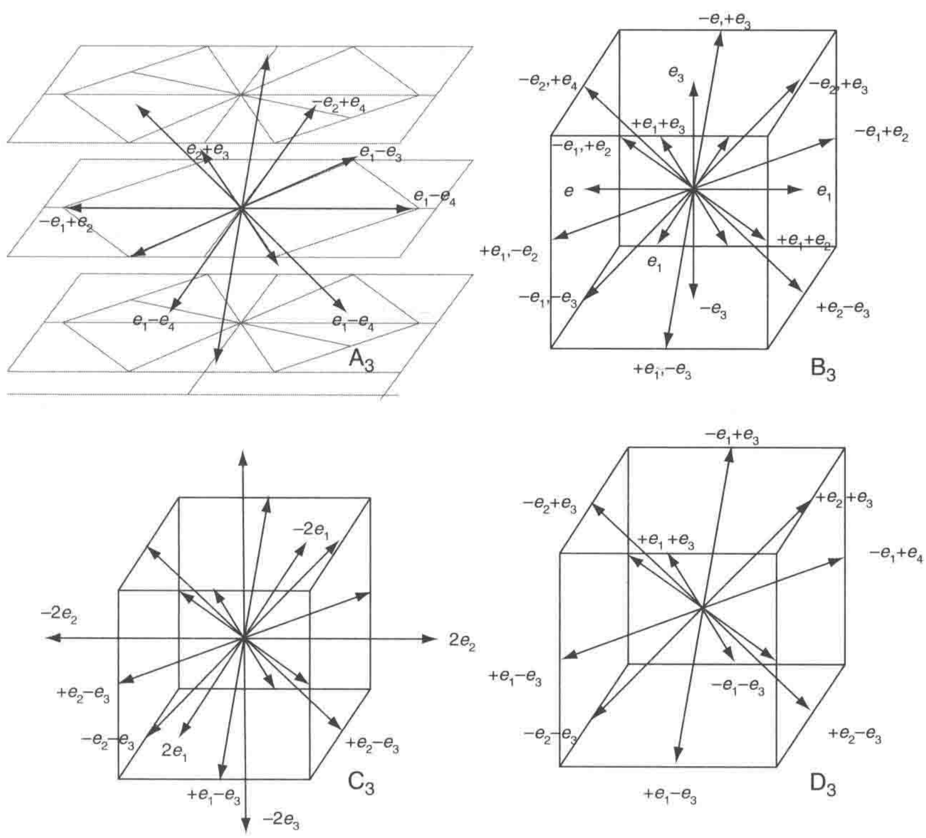


Figure 4 Rank-3 root spaces: $A_3, B_3, C_3, D_3 = A_3$.

Figure 4. The normalization factors (cf. point (9) above) are shown for the rank-2 root spaces in **Figure 3**.

Canonical Commutation Relations

The canonical commutation relations are expressed in terms of root vectors. The l operators in $\mathfrak{g}$ with the l-fold degenerate root vector 0 are $H_1, H_2, \ldots, H_l$. These l operators mutually commute. In a matrix Lie algebra, they can be taken as simultaneously commuting diagonal matrices. Associated with each nonzero root $\boldsymbol{\alpha} \neq 0$, there is exactly one basis vector, $E_{\boldsymbol{\alpha}}$, in $\mathfrak{g}$. The canonical commutation relations are expressed in terms of the roots as follows:

$$
\begin{aligned}
[H_i, H_j] &= 0 \qquad\qquad 1 \leq i, j \leq l \\
[H_i, E_{\boldsymbol{\alpha}}] &= \alpha_i E_{\boldsymbol{\alpha}} \\
[E_{\boldsymbol{\alpha}}, E_{-\boldsymbol{\alpha}}] &= \boldsymbol{\alpha} \cdot \boldsymbol{H} \\
[E_{\boldsymbol{\alpha}}, E_{\boldsymbol{\beta}}] &= \begin{cases} N_{\boldsymbol{\alpha\beta}} E_{\boldsymbol{\alpha}+\boldsymbol{\beta}} & \boldsymbol{\alpha}+\boldsymbol{\beta} \text{ a root} \\ 0 & \boldsymbol{\alpha}+\boldsymbol{\beta} \text{ not a root} \end{cases}
\end{aligned}
$$

The structure constants $N_{\boldsymbol{\alpha\beta}}$ are determined from a recursion relation derived from a chain of roots $\boldsymbol{\beta} - m\,\boldsymbol{\alpha}, \boldsymbol{\beta} - (m-1)\boldsymbol{\alpha}, \ldots, \boldsymbol{\beta} + (n-1)\boldsymbol{\alpha}, \boldsymbol{\beta} + n\boldsymbol{\alpha}$, where $\boldsymbol{\beta} - (m+1)\boldsymbol{\alpha}$ and $\boldsymbol{\beta} + (n+1)\,\boldsymbol{\alpha}$ are not roots (cf. **Figure 5**). The structure constants are

$$N^2_{\boldsymbol{\alpha},\boldsymbol{\beta}} = \tfrac{1}{2} n(1+m)(\boldsymbol{\alpha} \cdot \boldsymbol{\alpha})$$

The operators $\boldsymbol{H}$ and $E_{\boldsymbol{\alpha}}$ are often called diagonal and shift operators, respectively. They are generalizations of the shift operators J_3 and $J_\pm$ of angular momentum theory. The general idea is as follows. Since the operators H_i mutually commute, the matrices $\Gamma(H_i)$ representing these operators can be chosen as diagonal in any matrix representation.

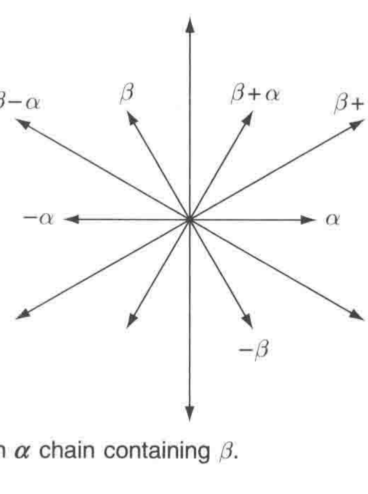


Figure 5 An α chain containing β.

The action of any of these operators on a basis vector in this representation is $H_i|\boldsymbol{m}\rangle = m_i|\boldsymbol{m}\rangle$. The operator E_α shifts the eigenvalue of $\boldsymbol{H}$ according to

$$\boldsymbol{H}(E_\alpha|\boldsymbol{m}\rangle) = ([\boldsymbol{H}, E_\alpha] + E_\alpha \boldsymbol{H})|\boldsymbol{m}\rangle = (\boldsymbol{\alpha} + \boldsymbol{m})(E_\alpha|\boldsymbol{m}\rangle)$$

In this sense the operators E_α act on basis vectors $|\boldsymbol{m}\rangle$ in such a way that the eigenvalue $\boldsymbol{m}$ is shifted by $\boldsymbol{\alpha}$ to $\boldsymbol{m} + \boldsymbol{\alpha}$.

For the simple classical Lie algebras, the roots can be expressed in terms of an orthogonal Euclidean basis set as shown in **Table 1** and **Figures 3** and **4** for the rank-2 and rank-3 root spaces. The roots for the five remaining inequivalent simple Lie algebras ("exceptional" algebras) are shown in **Table 2**.

The diagonal and shift operators for several of the classical Lie algebras can be related to bilinear products of boson or fermion creation and annihilation operators. For $\mathfrak{u}(n)$, the bilinear products $a_i^\dagger a_j$ are related to E_α with $\boldsymbol{\alpha} = \boldsymbol{e}_i - \boldsymbol{e}_j$, $1 \le i \ne j \le n$, and $H_i = a_i^\dagger a_i$. This holds for either boson or fermion operators. For $\mathfrak{sp}(2n; R)$, we have the identifications with bilinear products of boson operators as follows: $+\boldsymbol{e}_i + \boldsymbol{e}_j \leftrightarrow b_i^\dagger b_j^\dagger$, $+\boldsymbol{e}_i - \boldsymbol{e}_j \leftrightarrow b_i^\dagger b_j$, $-\boldsymbol{e}_i - \boldsymbol{e}_j \leftrightarrow b_i b_j$, and $H_i = b_i^\dagger b_i$. In particular, $+2\boldsymbol{e}_i \leftrightarrow b_i^{\dagger 2}$ and $-2\boldsymbol{e}_i \leftrightarrow b_i^2$. For $\mathfrak{so}(2n)$, we have the identifications with bilinear products of fermion operators as follows: $+\boldsymbol{e}_i + \boldsymbol{e}_j \leftrightarrow f_i^\dagger f_j^\dagger$, $+\boldsymbol{e}_i - \boldsymbol{e}_j \leftrightarrow f_i^\dagger f_j$, $-\boldsymbol{e}_i - \boldsymbol{e}_j \leftrightarrow f_i f_j$, and $H_i = f_i^\dagger f_i$. In particular, $f_i^\dagger f_i^\dagger = f_i^2 = 0$. These identifications make it a relatively simple matter to construct unitary matrix representations of the compact Lie groups SU(n) that are symmetric or antisymmetric, of USp($2n$) that are symmetric, and of SO($2n$) that are antisymmetric (bosons $\leftrightarrow$ symmetric, fermions $\leftrightarrow$ antisymmetric).

Dynkin Diagrams

Every root in a rank-l root space can be represented as a linear combination of l "basis roots." These basis roots can be chosen in such a way that all coefficients are integers. In fact, the basis roots can be chosen so that all linear combinations that are roots involve only positive integers (and zero) or only negative integers and zero. This comes about because every shift operator E_δ can be written as a multiple commutator

$$E_\delta \sim [E_\alpha, [E_\beta, E_\gamma]], \quad \boldsymbol{\delta} = \boldsymbol{\alpha} + \boldsymbol{\beta} + \boldsymbol{\gamma}$$

One simple way to construct such a basis set of fundamental roots is to construct an $(l-1)$-dimensional plane through the origin of the root space that contains no nonzero roots, and choose as l fundamental roots the l roots on one side of this hyperplane that are closest to it. For the classical simple Lie algebras, the fundamental roots are:

Root Space	α_1	α_2	α_{l-1}	α_l
A_{l-1}	$\boldsymbol{e}_1 - \boldsymbol{e}_2$	$\boldsymbol{e}_2 - \boldsymbol{e}_3$	$\boldsymbol{e}_{l-1} - \boldsymbol{e}_l$	
D_l	$\boldsymbol{e}_1 - \boldsymbol{e}_2$	$\boldsymbol{e}_2 - \boldsymbol{e}_3$	$\boldsymbol{e}_{l-1} - \boldsymbol{e}_l$	$\boldsymbol{e}_{l-1} + \boldsymbol{e}_l$
B_l	$\boldsymbol{e}_1 - \boldsymbol{e}_2$	$\boldsymbol{e}_2 - \boldsymbol{e}_3$	$\boldsymbol{e}_{l-1} - \boldsymbol{e}_l$	$+1\boldsymbol{e}_l$
D_l	$\boldsymbol{e}_1 - \boldsymbol{e}_2$	$\boldsymbol{e}_2 - \boldsymbol{e}_3$	$\boldsymbol{e}_{l-1} - \boldsymbol{e}_l$	$+2\boldsymbol{e}_l$

Table 1 Roots for the simple classical Lie groups and algebras

Group	*Algebra*	*Root space*	*Rank*	*Roots*	*Conditions*
SU(l)	$\mathfrak{su}(l)$	A_{l-1}	$l-1$	$+\boldsymbol{e}_i - \boldsymbol{e}_j$	$1 \le i \ne j \le l$
SO($2l$)	$\mathfrak{so}(2l)$	D_l	l	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$	$1 \le i < j \le l$
SO($2l+1$)	$\mathfrak{so}(2l+1)$	B_l	l	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$, $\pm\boldsymbol{e}_k$	$1 \le i < j, k \le l$
Sp(l) = USp($2l$)	$\mathfrak{sp}(l) = \mathfrak{usp}(2l)$	C_l	l	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$, $\pm 2\boldsymbol{e}_k$	$1 \le i < j, k \le l$

Table 2 Roots for the simple exceptional Lie algebras

Root space	*Rank*	*Dimension*	*Roots*	*Conditions*
G_2	2	14	$+\boldsymbol{e}_i - \boldsymbol{e}_j$ $\pm[(\boldsymbol{e}_i + \boldsymbol{e}_j) - 2\boldsymbol{e}_k]$	$1 \le i \ne j \ne k \le 3$
F_4	4	52	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$, $\pm 2\boldsymbol{e}_i$ $\pm\boldsymbol{e}_1 \pm \boldsymbol{e}_2 \pm \boldsymbol{e}_3 \pm \boldsymbol{e}_4$	$1 \le i < j \le 4$
E_6	6	78	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$ $\frac{1}{2}(\pm\boldsymbol{e}_1 \pm \boldsymbol{e}_2 \pm \boldsymbol{e}_3 \pm \boldsymbol{e}_4 \pm \boldsymbol{e}_5) \pm \frac{\sqrt{3}}{4}\boldsymbol{e}_6$	$1 \le i < j \le 5$ a
E_7	7	133	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$ $\frac{1}{2}(\pm\boldsymbol{e}_1 \pm \boldsymbol{e}_2 \pm \boldsymbol{e}_3 \pm \boldsymbol{e}_4 \pm \boldsymbol{e}_5 \pm \boldsymbol{e}_6) \pm \frac{\sqrt{2}}{4}\boldsymbol{e}_7$	$1 \le i < j \le 6$ b
E_8	8	248	$\pm\boldsymbol{e}_i \pm \boldsymbol{e}_j$ $\frac{1}{2}(\pm\boldsymbol{e}_1 \pm \boldsymbol{e}_2 \pm \boldsymbol{e}_3 \pm \boldsymbol{e}_4 \pm \boldsymbol{e}_5 \pm \boldsymbol{e}_6 \pm \boldsymbol{e}_7 \pm \boldsymbol{e}_8)$	$1 \le i < j \le 8$ a

[a]Even number of + signs.

[b]Even number of + signs within bracket.

All roots in the rank-2 root spaces have been expressed in terms of both two orthogonal vectors and two fundamental roots in **Figure 3**.

If α_i and α_j are fundamental roots, their inner product is zero or negative

$$\cos(\alpha_i, \alpha_j) = 0, -\sqrt{\frac{1}{4}}, -\sqrt{\frac{2}{4}}, -\sqrt{\frac{3}{4}}$$

This information has been used to classify the root spaces of the inequivalent simple Lie algebras (over C). The procedure is as follows. Each of the l fundamental roots in a rank-l root space is represented by a dot in a plane. Dots representing roots α_i and α_j are connected by n_{ij} lines, where $\cos(\alpha_i, \alpha_j) = -\sqrt{n_{ij}/4}$. Orthogonal roots are not connected by any lines. Such diagrams are called Dynkin diagrams. Disconnected Dynkin diagrams describe semisimple Lie algebras. Connected Dynkin diagrams classify simple Lie algebras.

The properties of Dynkin diagrams arise from two simple observations:

O1: The root space is positive definite.

O2: If u is a unit vector and v_i are an orthonormal set of vectors,

$$\sum (u \cdot v_i)^2 \leq 1$$

These two observations lead to three important properties of Dynkin diagrams.

D1: There are no loops. If α_i $(i = 1, 2, \ldots, k)$ are in a loop, then there are at least as many lines as vertices. With $u_i = \alpha_i/|\alpha_i|$,

$$\left(\sum_{i=1}^{k} u_i, \sum_{j=1}^{k} u_j \right) = k + 2\sum_{i<j}^{k} u_i \cdot u_j > 0$$

Since $2u_i \cdot u_j \leq -1$ if $u_i \cdot u_j \neq 0$, there cannot be as many lines as vertices.

D2: The number of lines connected to any node is <4. If α_i are connected to v, then with $u_i = \alpha_i/|\alpha_i|$,

$$\sum (v \cdot u_i)^2 = \sum n_i/4 < 1$$

since v is linearly independent of the α_i.

D3: A simple chain connecting any two nodes can be shrunk. If the original diagram is allowed, the shrunk diagram is also allowed, and conversely. Since the shrunk diagram in **Figure 6** violates $D2$, the original is not an allowed Dynkin diagram.

According to these results, the maximum number of lines that can be attached to a vertex is three. If a vertex is attached to three lines, it can be connected to three (one line each) other vertices, two (two plus

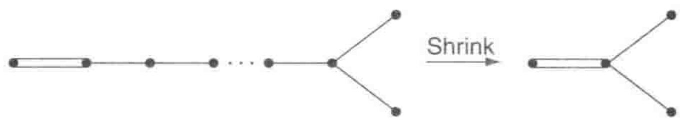


Figure 6 A chain with single links can be removed from a diagram. If the original is an allowed Dynkin diagram, the shrunk diagram is also allowed, and conversely.

one) other vertices, or only one other vertex (all three lines). This last case describes Dynkin diagram G_2 (cf. **Figures 3** and **5**).

The only remaining possibilities are shown in **Figure 7**.

For diagrams of type (B, C, F) we define vectors

$$u = \sum_{i=1}^{p} iu_i \qquad v = \sum_{j=1}^{q} jv_j$$

where as usual u_i, v_j are unit vectors $\alpha_k/|\alpha_k|$. The Schwartz inequality applied to u and v leads to the inequality

$$\left(1 + \frac{1}{p}\right)\left(1 + \frac{1}{q}\right) > 2$$

The solutions with $p \geq q$ are

p	q	Root space	Constraint
arbitrary	1	B_l, C_l	$i = p + 1$
2	2	F_4	

For diagrams of type (D, E), we define vectors

$$u = \sum_{i=1}^{p-1} iu_i, \qquad v = \sum_{j=1}^{q-1} jv_j, \qquad w = \sum_{k=1}^{r-1} kw_k$$

where as usual u_i, v_j, w_k are unit vectors $\alpha_m/|\alpha_m|$. With similar arguments, we obtain the inequality

$$\frac{1}{p} + \frac{1}{q} + \frac{1}{r} > 2$$

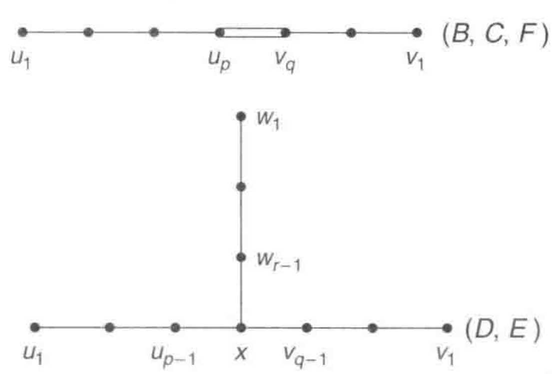


Figure 7 The only remaining candidate Dynkin diagrams have either two vertices (B, C, F) or one vertex (D, E) connected to three lines.

The solutions with $p \geq q \geq r$ are

p	*q*	*r*	*Root space*	*Regular Euclidean solid*
arbitrary	2	2	$D_p + 2$	
3	3	2	E_6	Tetrahedron
4	3	2	E_7	Cube–octahedron
5	3	2	E_8	Icosahedron–dodecahedron

All allowed Dynkin diagrams are shown in **Figure 8**. In these diagrams roots making an angle of 120° with each other (joined by single lines) have equal length. Roots joined by double lines or triple lines have different lengths. The arrows on double lines indicated the shorter and longer roots. Arrows point to longer roots. The root space G_2 and F_4 are self-dual, so it does not matter which way the arrow points.

Coxeter–Dynkin diagrams also appear in classical geometry and catastrophe theory.

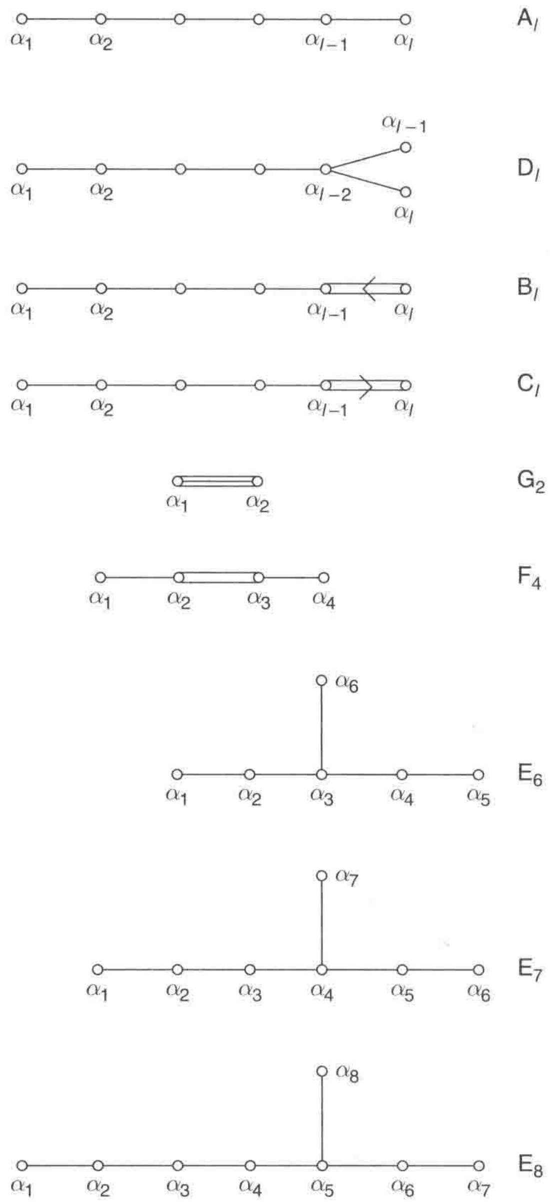


Figure 8 Four infinite series (A_l, D_l, B_l, C_l) of Dynkin diagrams exist and correspond to the classical simple Lie groups (SU $(l+1)$, SO$(2l)$, SO$(2l+1)$, USp$(2l)$). The five exceptional Dynkin diagrams include a short finite series ($E_l, l = 6, 7, 8$), F_4, and G_2.

Real Forms

The metric tensor $g_{\mu\nu}$ for a simple Lie algebra (over C) in the canonical basis $\boldsymbol{H}, E_{\boldsymbol{\alpha}}$ is

$$g \to \left[\begin{array}{cccc|cccc} 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & & & & \\ \hline & & & & 0 & 1 & & \\ & & & & 1 & 0 & & \\ & & & & & & 0 & 1 \\ & & & & & & 1 & 0 \\ & & & & & & & \ddots \end{array}\right] \begin{array}{c} H_1 \\ H_2 \\ \vdots \\ H_l \\ E_{+\alpha} \\ E_{-\alpha} \\ E_{+\beta} \\ E_{-\beta} \\ \vdots \end{array} \qquad [2]$$

In this basis, the Lie algebra decomposes into positive- and negative-definite subspaces according to

$$\mathfrak{g} = \mathfrak{g}_+ + \mathfrak{g}_-$$

$$\begin{array}{lll} \mathfrak{g}_+ \text{ spanned by} & H_i, & (E_{+\alpha} + E_{-\alpha})/\sqrt{2} \\ \mathfrak{g}_- \text{ spanned by} & & (E_{+\alpha} - E_{-\alpha})/\sqrt{2} \end{array}$$

The choice of basis suggested above diagonalizes the Cartan–Killing form in eqn [2]: $g \to I_{p,q}$, with $p = l + (1/2)(n - l)$ positive values +1 on the diagonal and $q = (1/2)(n - l)$ values –1 on the diagonal. The trace of this matrix is the trace of g: $+l$.

An arbitrary element in this (complex) Lie algebra is a linear superposition of the form

$$X = \sum_i h^i H_i + \sum_{\alpha \neq 0} e^{\alpha} E_{\alpha} \qquad [3]$$

where all n coefficients h^i, e^{α} are complex. If all these coefficients are taken real, the resulting Lie algebra closes under commutation and describes a noncompact Lie group. The subalgebra describing the maximal compact subgroup is spanned by the

linear combinations $(E_{+\alpha} - E_{-\alpha})/\sqrt{2}$. The remaining operators exponentiate to a noncompact coset

$$\mathrm{EXP}\left\{h^i H_i + e_+^\alpha (E_{+\alpha} + E_{-\alpha})/\sqrt{2}\right\}$$

which is topologically equivalent to $R^K, K = l + (1/2)(n-l) = (1/2)(n+l)$. Of all the real forms of the complex Lie algebra described by this set of canonical commutation relations (or root space, or Dynkin diagram), this is the least compact real form.

The compact real form is obtained from [3] by taking linear combinations

$$X = \sum_i \mathrm{i}h^i H_i + \sum_{\alpha \neq 0} \mathrm{i}e_+^\alpha (E_{+\alpha} + E_{-\alpha})/\sqrt{2} + \sum_{\alpha \neq 0} e_-^\alpha (E_{+\alpha} - E_{-\alpha})/\sqrt{2}$$

where $h^i, e_+^\alpha, e_-^\alpha$ are real. The compact real forms of the simple Lie algebras are:

Root space	*Group*
$A_l - 1$	SU(l)
D_l	SO($2l$)
B_l	SO($2l + 1$)
C_l	USp($2l$) = Sp(l)

If the imaginary factor i is absorbed into the Cartan–Killing metric, this metric is diagonal, all matrix elements are –1, the trace of this form is $-n$, and the linear combinations for X are real.

Every complex simple Lie algebra (i.e., simple Lie algebra over C) has a spectrum of inequivalent real forms. These can all be obtained from the compact real form by an analog of Minkowski's "rotation trick," derived by Cartan. Cartan introduced a metric-preserving linear mapping ("involutive automorphism") $T : \mathfrak{g} \to \mathfrak{g}$ with the property $T^2 = I$ and $(TX, TY) = (X, Y)$, with $X, Y \in \mathfrak{g}$. The operator T has eigenvalues ± 1 and induces a decomposition ("Cartan decomposition") in $\mathfrak{g}$ as follows:

$$\begin{array}{cccccc} & T(\mathfrak{g}) & = & T(\mathfrak{k}) & + & T(\mathfrak{p}) \\ \mathfrak{g} = \mathfrak{k} + \mathfrak{p} & & & \downarrow & & \downarrow \\ & & & \mathfrak{k} & - & \mathfrak{p} \end{array}$$

As a result, the subspaces $\mathfrak{k}$ and $\mathfrak{p}$ are orthogonal. The subspaces obey the following commutation and inner-product properties:

$$\begin{array}{ll} [\mathfrak{k}, \mathfrak{k}] \subseteq \mathfrak{k}, & (\mathfrak{k}, \mathfrak{k}) < 0 \\ [\mathfrak{k}, \mathfrak{p}] \subseteq \mathfrak{p}, & (\mathfrak{k}, \mathfrak{p}) = 0 \\ [\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{k}, & (\mathfrak{p}, \mathfrak{p}) < 0 \end{array}$$

Under the analytic continuation $\mathfrak{p} \to \mathrm{i}\mathfrak{p}$, the compact Lie algebra $\mathfrak{g}$ is rotated to a noncompact Lie algebra $\mathfrak{g}'$ whose commutation relations and inner-product properties are

$$\mathfrak{g} = \mathfrak{k} + \mathfrak{p} \quad \to \quad \mathfrak{g}' = \mathfrak{k} + \mathfrak{p}'$$

$$\begin{array}{ll} [\mathfrak{k}, \mathfrak{k}] \subseteq \mathfrak{k}, & (\mathfrak{k}, \mathfrak{k}) < 0 \\ [\mathfrak{k}, \mathfrak{p}'] \subseteq \mathfrak{p}', & (\mathfrak{k}, \mathfrak{p}') = 0 \\ [\mathfrak{p}', \mathfrak{p}'] \subseteq \mathfrak{k}, & (\mathfrak{p}', \mathfrak{p}') > 0 \end{array}$$

The maximal compact subalgebra of $\mathfrak{g}'$ is $\mathfrak{k}$. The subspace $\mathfrak{p}'$ exponentiates to a simply connected submanifold on which the Cartan–Killing metric is positive definite. This manifold is topologically equivalent to R^K, $K = \dim \mathfrak{p}$. It is not geometrically equivalent to R^K once an invariant metric is placed on it.

Three linear mappings that satisfy $T^2 = I$ suffice to generate all real forms of all the simple classical Lie algebras.

Block Matrix Decomposition

The compact Lie algebra $\mathfrak{u}(n; F)$ has a block submatrix decomposition ($n = p + q$):

$$\mathfrak{u}(n; F) = \begin{bmatrix} A_p & 0 \\ 0 & A_q \end{bmatrix} + \begin{bmatrix} 0 & +B \\ -B^\dagger & 0 \end{bmatrix}$$

where $A_p^\dagger = -A_p, A_q^\dagger = -A_q$ and B is an arbitrary $p \times q$ matrix over F. Under the map

$$T(\mathfrak{g}) = I_{p,q}\mathfrak{g}I_{p,q}, \ I_{p,q} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}$$

the diagonal subspace

$$\begin{bmatrix} A_p & 0 \\ 0 & A_q \end{bmatrix}$$

has eigenvalue +1 and the off-diagonal subspace

$$\begin{bmatrix} 0 & +B \\ -B^\dagger & 0 \end{bmatrix}$$

has eigenvalue –1. Under the Cartan rotation

$$\mathfrak{u}(n; F) \to \mathfrak{u}(p, q; F) = \begin{bmatrix} A_p & 0 \\ 0 & A_q \end{bmatrix} + \begin{bmatrix} 0 & +B \\ +B^\dagger & 0 \end{bmatrix}$$

The real forms of the classical Lie groups obtained in this way are

$$D_n, B_n$$

$$\begin{matrix} SO(2n) & & \\ & \rightarrow & SO(p,q) \\ SO(2n+1) & & \end{matrix}$$

$$A_{n-1}$$
$$SU(n) \rightarrow SU(p,q)$$

$$C_n$$
$$Sp(n) \rightarrow Sp(p,q)$$
$$USp(2n) \rightarrow USp(2p,2q)$$

Subfield Restriction

The Lie algebra $\mathfrak{su}(n)$ of complex traceless anti-Hermitian matrices has a subalgebra $\mathfrak{so}(n)$ of real antisymmetric matrices. The algebra $\mathfrak{su}(n)$ can be expressed in terms of real $n \times n$ antisymmetric matrices A_n and traceless symmetric matrices S_n:

$$\mathfrak{su}(n) = \mathfrak{so}(n) + [\mathfrak{su}(n) - \mathfrak{so}(n)] = A_n + iS_n$$

The Cartan rotation is

$$\mathfrak{su}(n) \rightarrow \mathfrak{sl}(n;R) = \mathfrak{so}(n) + i[\mathfrak{su}(n) - \mathfrak{so}(n)] = A_n + S_n$$

The classical Lie group generated by this transformation is $SL(n;R)$.

A similar rotation can be carried out on unitary matrices over the quaternion field, $\mathfrak{u}(n;Q) = \mathfrak{sp}(n)$. This algebra contains the subalgebra $\mathfrak{u}(n)$ in which quaternions $q = q_0 + \mathcal{I}q_1 + \mathcal{J}q_2 + \mathcal{K}q_3$ are restricted to complex numbers $q = q_0 + iq_1$. There is a natural decomposition

$$\mathfrak{sp}(n) = \mathfrak{u}(n) + [\mathfrak{sp}(n) - \mathfrak{u}(n)]$$

It is useful at this point to replace each quaternion matrix element by a 2×2 complex matrix: $\mathfrak{sp}(n) \rightarrow \mathfrak{usp}(2n)$. This is a unitary representation of the symplectic algebra. Replacing the complex matrix elements in $\mathfrak{u}(n)$ by 2×2 real matrices simultaneously generates a real matrix representation of $\mathfrak{u}(n)$ named $\mathfrak{ou}(2n)$. This is an orthogonal representation of the unitary algebra. The decomposition above is

$$\mathfrak{sp}(n) \rightarrow \mathfrak{u}(n) + [\mathfrak{sp}(n) - \mathfrak{u}(n)] \rightarrow \mathfrak{ou}(2n) + [\mathfrak{usp}(2n) - \mathfrak{ou}(2n)] = A_{2n} + iS_{2n}$$

where as before A_{2n} and S_{2n} are $2n \times 2n$ antisymmetric and symmetric matrices. The Cartan rotation maps this to $\mathfrak{sp}(2n;R)$,

$$\mathfrak{usp}(2n) \rightarrow \mathfrak{sp}(2n;R) = A_{2n} + S_{2n}$$

The classical Lie group generated in this way is $Sp(2n;R)$. Matrices in this group satisfy the quadratic constraint $M^tGM = G, G^t = -G, \det(G) \neq 0$. The real symplectic groups leave invariant Hamilton's equations of motion: $dp_i/dt = -\partial H/\partial q_i$, $dq_i/dt = +\partial H/\partial p_i$.

Field Embeddings

The image of $\mathfrak{u}(n) \rightarrow \mathfrak{ou}(2n)$ consists of a set of $2n \times 2n$ antisymmetric matrices of dimension n^2. These matrices form a subset of $\mathfrak{so}(2n)$, which consists of $2n \times 2n$ antisymmetric matrices of dimension $2n(2n-1)/2$. As a result, $\mathfrak{ou}(2n)$ is a subalgebra in $\mathfrak{so}(2n)$. Thus, $\mathfrak{ou}(2n) \sim \mathfrak{k}$ and $\mathfrak{so}(2n) \sim \mathfrak{g}$ and we have a Cartan decomposition

$$\begin{matrix} \mathfrak{so}(2n) = \mathfrak{ou}(2n) + [\mathfrak{so}(2n) - \mathfrak{ou}(2n)] \\ \downarrow \qquad\qquad \downarrow \\ \mathfrak{ou}(2n) + i[\mathfrak{so}(2n) - \mathfrak{ou}(2n)] = \mathfrak{so}^*(2n) \end{matrix}$$

In the same way, the image of $\mathfrak{sp}(2n) \rightarrow \mathfrak{usp}(2n)$ consists of an $n(2n+1)$-dimensional set of $2n \times 2n$ anti-Hermitian matrices. This is a subset of $\mathfrak{su}(2n)$, which has dimension $(2n)^2 - 1$. It is also a subalgebra of $\mathfrak{su}(2n)$. Thus, $\mathfrak{usp}(2n) \sim \mathfrak{k}$ and $\mathfrak{su}(2n) \sim \mathfrak{g}$, so we have a Cartan decomposition

$$\begin{matrix} \mathfrak{su}(2n) = \mathfrak{usp}(2n) + [\mathfrak{su}(2n) - \mathfrak{usp}(2n)] \\ \downarrow \qquad\qquad \downarrow \\ \mathfrak{usp}(2n) + i[\mathfrak{su}(2n) - \mathfrak{usp}(2n)] = \mathfrak{su}^*(2n) \end{matrix}$$

These real forms are summarized in **Table 3**.

Table 3 Real forms of the simple classical Lie algebras

Mapping	*Real form*	*Maximal compact subalgebra*	*Root space*	*Condition*
Block submatrix	$\mathfrak{so}(p,q)$	$\mathfrak{so}(p) + \mathfrak{so}(q)$	D_n	$p+q=2n$
	$\mathfrak{so}(p,q)$	$\mathfrak{so}(p) + \mathfrak{so}(q)$	B_n	$p+q=2n+1$
	$\mathfrak{su}(p,q)$	$\mathfrak{u}(1) + \mathfrak{su}(p) + \mathfrak{su}(q)$	A_{n-1}	$p+q=n$
	$\mathfrak{sp}(p,q) = \mathfrak{usp}(2p,2q)$	$\mathfrak{usp}(2p) + \mathfrak{usp}(2p)$	C_n	$p+q=n$
Subfield restriction	$\mathfrak{sl}(n;R)$	$\mathfrak{so}(n)$	A_{n-1}	
	$\mathfrak{sp}(2n;R)$	$\mathfrak{u}(n)$	C_n	
Field embedding	$\mathfrak{so}^*(2n)$	$\mathfrak{u}(n)$	D_n	
	$\mathfrak{su}^*(2n)$	$\mathfrak{sp}(n) = \mathfrak{usp}(2n)$	A_{2n-1}	

Table 4 Equivalence among real forms of the simple classical Lie algebras

A_1	$= B_1$	$= C_1$	χ
$\mathfrak{su}(2)$	$= \mathfrak{so}(3)$	$= \mathfrak{sp}(1) = \mathfrak{usp}(2)$	-3
$\mathfrak{su}(1,1) = \mathfrak{sl}(2;R)$	$= \mathfrak{so}(2,1)$	$= \mathfrak{sp}(2;R)$	$+1$
D_2	$= A_1$	$+ A_1$	χ
$\mathfrak{so}(4)$	$= \mathfrak{so}(3)$	$+ \mathfrak{so}(3)$	-6
$\mathfrak{so}^*(4)$	$= \mathfrak{so}(3)$	$+ \mathfrak{so}(2,1)$	-2
$\mathfrak{so}(3,1)$	$= \mathfrak{sl}(2;C)$		0
$\mathfrak{so}(2,2)$	$= \mathfrak{so}(2,1)$	$+ \mathfrak{so}(2,1)$	$+2$
B_2	$= C_2$		χ
$\mathfrak{so}(5)$	$= \mathfrak{sp}(2) = \mathfrak{usp}(4)$		-10
$\mathfrak{so}(4,1)$	$= \mathfrak{sp}(1,1) = \mathfrak{usp}(2,2)$		-2
$\mathfrak{so}(3,2)$	$= \mathfrak{sp}(4;R)$		$+2$
D_3	$= A_3$		χ
$\mathfrak{so}(6)$	$= \mathfrak{su}(4)$		-15
$\mathfrak{so}(5,1)$	$= \mathfrak{su}^*(4)$		-5
$\mathfrak{so}^*(6)$	$= \mathfrak{su}(3,1)$		-3
$\mathfrak{so}(4,2)$	$= \mathfrak{su}(2,2)$		$+1$
$\mathfrak{so}(3,3)$	$= \mathfrak{sl}(4;R)$		$+3$

The root spaces $A_1[\mathrm{SU}(2)], B_1[\mathrm{SO}(3)]$, and $C_1[\mathrm{U}(1;Q) \simeq \mathrm{USp}(2;C)]$ are equivalent. As a result, the different real forms of their complex extensions are related to each other. Similar remarks hold for the real forms of $B_2 = C_2$, $D_2 = A_1 + A_1$, and $D_3 = A_3$. The relations among these real forms are summarized in **Table 4**. This table is useful in inferring "spinor representations" among classical groups. Thus, SO(3) has spinor representations based on SU(2) and Sp(1); SO(4) has spinor representations based on $\mathrm{SU}(2) \times \mathrm{SU}(2)$; SO(5) has spinor representations based on USp(4); and SO(6) has spinor representations based on SU(4).

For completeness, the real forms for the exceptional Lie algebras are collected in **Table 5**.

Real forms of the complex extension of a simple Lie algebra are almost uniquely distinguished by an index. This is the trace of the Cartan–Killing form [2], once the appropriate factors of i have been absorbed into it. If n_c is the dimension of the maximal compact subgroup, $\chi = \mathrm{tr}(g) = +1(n - n_c) - 1(n_c) = n - 2n_c$. The index ranges from $-n$ for the compact real form (for which $n_c = n$) to $+l$ for the least compact real form.

Riemannian Symmetric Spaces

Exponentiation lifts Lie algebras to Lie groups and subspaces in Lie algebras into submanifolds in Lie groups. In particular, exponentiation of a Cartan decomposition

Table 5 Real forms of the exceptional Lie algebras

		Maximal compact subgroup	
Root space	*Class*$_{Rank(Character)}$	*Root space*	*Dimension*
G_2	$G_{2(-14)}$	G_2	14
	$G_{2(+2)}$	$A_1 + A_1$	6
F_4	$F_{4(-52)}$	F_4	52
	$F_{4(-20)}$	B_4	36
	$F_{4(+4)}$	$C_3 + A_1$	24
E_6	$E_{6(-78)}$	E_6	78
	$E_{6(-26)}$	F_4	52
	$E_{6(-14)}$	$D_5 + D_1$	46
	$E_{6(+2)}$	$A_5 + A_1$	38
	$E_{6(+6)}$	C_4	36
E_7	$E_{7(-133)}$	E_7	133
	$E_{7(-25)}$	$E_6 + D_1$	79
	$E_{7(-5)}$	$D_6 + A_1$	69
	$E_{7(+7)}$	A_7	63
E_8	$E_{8(-248)}$	E_8	248
	$E_{8(-24)}$	$E_7 + A_1$	136
	$E_{8(+8)}$	D_8	120

$$\begin{array}{ccccc} \mathfrak{g} & = & \mathfrak{k} & + & \mathfrak{p} \\ \downarrow & & \downarrow & & \downarrow \\ G & = & K & \times & (P = G/K) \end{array}$$

lifts the subspace $\mathfrak{p}$ to the quotient $(P = G/K)$.

A metric may be defined on the Lie group G as follows. Define the distance between the identity and some nearby point $g(\epsilon) = \mathrm{EXP}(\epsilon X) = \mathrm{EXP}(\delta x^i X_i)$ by

$$ds^2(0) = G_{rs}\delta x^r \delta x^s$$

Move I and $g(\epsilon)$ to the neighborhood of any point $g(x) \in G$ by left multiplication: $g(x)I \to g(x)$, $g(x)g(\delta x^i X_i) \to g((x + dx)^i X_i)$. The infinitesimals $dx^i(x)$ at x (defined by $g(x)$) and $\delta x^i = dx^i(0)$ at I are linearly related,

$$\delta x^i = M^i{}_j(x)\, dx^j(x)$$

By requiring that the distance ds between I and $g(\delta x^i X_i)$ at the identity be the same as the distance between $g(x^i X_i)I$ and $g(x^i X_i)g(\delta x^i X_i) = g((x + dx)^i X_i)$ at $g(x^i X_i)$ leads to the condition

$$\begin{aligned} ds^2 &= G_{rs}(0)\delta x^r \delta x^s \\ &= G_{rs}(0)M^r{}_i(x)M^s{}_j(x)\, dx^i(x)\, dx^j(x) \\ &= G_{ij}(x)\, dx^i(x)\, dx^j(x) \end{aligned}$$

An invariant metric $G(x)$ over the Lie group G is defined by

$$\begin{aligned} G_{ij}(x) &= G_{rs}(0)M^r{}_i(x)M^s{}_j(x) \\ G(x) &= M^t(x)G(0)M(x) \end{aligned}$$

It is useful to identify $G(0)$ with the Cartan–Killing inner product on $\mathfrak{g}$. Since $M(x)$ is nonsingular, the signature of $G(x)$ is invariant over the group.

The invariant metric on G can be restricted to subspaces $K \subset G$ and $P = G/K \subset G$. The signature on these subspaces is the same as the signature on the subspaces $\mathfrak{k}$ and $\mathfrak{p}$ in $\mathfrak{g}$. Thus, if G is compact, the invariant metric is negative definite on K and on $P = G/K$ and positive definite on the analytically continued space $P' = G'/K$. In short, it is definite (negative, positive) on P, P'. These spaces are Riemannian spaces and they are globally symmetric. They have been investigated by studying the properties of the secular equation of the Lie algebra $\mathfrak{g}$, restricted to the subspace $\mathfrak{p}$:

$$\det[R(p^i P_i) - \lambda I] = \sum_j (-\lambda)^{n-j} \hat{\phi}_j(p) = 0 \qquad [4]$$

where the P_i are basis vectors that span $\mathfrak{p}$. The coefficients $\hat{\phi}_j(p)$ in the secular equation [4] for Riemannian symmetric spaces are related to the coefficients $\phi_j(x)$ in the secular equation [1] for Lie algebras. A rank for the Riemannian symmetric space $P = \mathrm{EXP}(\mathfrak{p})$ can be defined from the secular equation following exactly the prescription followed for the Lie algebra $\mathfrak{g}$. The rank of the Riemannian symmetric space $P = \mathrm{EXP}(\mathfrak{p})$ is

1. the number of functionally independent coefficients $\hat{\phi}_j(p)$ in the secular equation;
2. the number of independent roots of the secular equation;
3. the dimension of the maximal Euclidean subspace in P; and
4. the number of independent (Laplace–Beltrami) operators that commute with all displacement operators P_i: $\Delta_j(P) = \hat{\phi}_j(p^i \to P_i)$.

Rank-1 Riemannian symmetric spaces are isotropic as well as homogeneous.

Tables 3 and **5** contain all the information required to enumerate all the classical and exceptional Riemannian symmetric spaces. All the classical Riemannian symmetric spaces are tabulated in **Table 6**. The exceptional Riemannian symmetric spaces can be constructed from the information in **Table 5** following the procedure used to construct **Table 6** from **Table 3**.

As particular examples of Riemannian symmetric spaces we consider the compact spaces $\mathrm{SO}(p+q)/[\mathrm{SO}(p) \times \mathrm{SO}(q)]$ and their noncompact counterparts $\mathrm{SO}(p,q)/[\mathrm{SO}(p) \times \mathrm{SO}(q)]$. These spaces have rank $\min(p,q)$, dimension pq, and can be represented explicitly in matrix form as

$$\left[\begin{array}{c|c} 0 & X \\ \hline \sigma X^t & 0 \end{array}\right] \to \mathrm{EXP}\left[\begin{array}{c|c} 0 & X \\ \hline \sigma X^t & 0 \end{array}\right] = \left[\begin{array}{c|c} D_p & Y \\ \hline \sigma Y^t & D_q \end{array}\right]$$

Here X is a $p \times q$ matrix and $\sigma = +1$ for the noncompact case and -1 for the compact case. The block diagonal matrices D_p and D_q are defined from the metric-preserving conditions ($M^t I_{p+q} M = I_{p+q}$, $M^t I_{p,q} M = I_{p,q}$)

$$D_p^2 = I_p + \sigma Y Y^t, \qquad D_q^2 = I_q + \sigma Y^t Y$$

The pq coordinates in the Riemannian symmetric spaces can be taken as the pq elements of the submatrix Y.

These Riemannian symmetric spaces can be treated as algebraic submanifolds in $R^K, K = pq + (1/2)q(q+1)$. The K coordinates on R^K can be identified with the pq matrix elements of Y and the $(1/2)q(q+1)$ matrix elements of the real symmetric matrix D_q. These coordinates obey the $(1/2)q(q+1)$ algebraic constraints defined by

$$D_q^2 - \sigma Y^t Y = I_q$$

For SO(3)/SO(2) and SO(2,1)/SO(2), this condition is determined from the matrix

$$\left[\begin{array}{c|c} \left[I_2 + \begin{pmatrix} \sigma x & \sigma y \end{pmatrix} \begin{bmatrix} x \\ y \end{bmatrix}\right]^{1/2} & \begin{matrix} x \\ y \end{matrix} \\ \hline \begin{matrix} \sigma x & \sigma y \end{matrix} & z \end{array}\right] \quad \text{to be}$$

$$z^2 - \sigma(x^2 + y^2) = 1$$

Table 6 All classical Riemannian symmetric spaces

Root space	*Quotient*	*Dimension*	*Rank*	χ
A_{p+q-1}	$\mathrm{SU}(p,q)/\mathrm{S}[\mathrm{U}(p) \otimes \mathrm{U}(q)]$	$2pq$	$\min(p,q)$	$1-(p-q)^2$
A_{n-1}	$\mathrm{SL}(n;R)/\mathrm{SO}(n)$	$\frac{1}{2}(n+2)(n-1)$	$n-1$	$n-1$
A_{2n-1}	$\mathrm{SU}^*(2n)/\mathrm{USp}(2n)$	$(2n+1)(n-1)$	$n-1$	$-2n-1$
B_{p+q}	$\mathrm{SO}(p,q)/\mathrm{SO}(p) \otimes \mathrm{SO}(q)$	pq	$\min(p,q)$	$pq - \frac{1}{2}p(p-1) - \frac{1}{2}q(q-1)$
D_{p+q}	$\mathrm{SO}(p,q)/\mathrm{SO}(p) \otimes \mathrm{SO}(q)$	pq	$\min(p,q)$	$pq - \frac{1}{2}p(p-1) - \frac{1}{2}q(q-1)$
D_n	$\mathrm{SO}^*(2n)/\mathrm{U}(n)$	$n(n-1)$	$n/2$	$-n$
C_{p+q}	$\mathrm{USp}(2p,2q)/\mathrm{USp}(2p) \otimes \mathrm{USp}(2q)$	$4pq$	$\min(p,q)$	$-2(p-q)^2 - (p+q)$
C_n	$\mathrm{Sp}(2n;R)/\mathrm{U}(n)$	$n(n+1)$	n	$+n$

For $\sigma = -1$, the space is the sphere S^2 defined by $z^2 + (x^2 + y^2) = 1$. For $\sigma = +1$, the space is the two-sheeted hyperboloid H_2^2 defined by $z^2 - (x^2 + y^2) = 1$. More specifically, it is the upper sheet containing $(0, 0, 1)$ of the two-sheeted hyperboloid. The second sheet occurs in the coset O(2,1)/SO(2). The symmetric spaces $SO(n+1)/SO(n)$ and $SO(n,1)/SO(n)$ are the sphere S^n and the upper sheet of the two-sheeted hyperboloid H_{2+}^n. Both have dimension n and rank 1. The spaces are simply connected, homogeneous, and isotropic.

For $SO(4,2)/SO(4) \times SO(2)$, the eight-dimensional algebraic manifold is defined by the three constraints in R^{11}:

$$\begin{bmatrix} y_9 & y_{10} \\ y_{10} & y_{11} \end{bmatrix}^2 - \sigma \begin{bmatrix} y_1 & y_2 & y_3 & y_4 \\ y_5 & y_6 & y_7 & y_8 \end{bmatrix} \begin{bmatrix} y_1 & y_5 \\ y_2 & y_6 \\ y_3 & y_7 \\ y_4 & y_8 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The compact analytically continued space $SO(6)/SO(4) \times SO(2)$ is obtained by setting $\sigma = -1$. These spaces have dimension 8 and rank 2. They are homogeneous but not isotropic. For each, there are "two inequivalent directions." There are two independent Laplace–Beltrami operators on these spaces, one quadratic and one quartic.

The complete list of globally symmetric pseudo-Riemannian symmetric spaces can be constructed almost as easily. Two linear operators, T_1 and T_2, are introduced that obey $T_1^2 = I, T_2^2 = I, T_1T_2 = T_2T_1 \neq I$. The two are used to split $\mathfrak{g}$ into subspaces

$$T_1\, \mathfrak{g}_{\sigma\tau} = \sigma\, \mathfrak{g}_{\sigma\tau}, \qquad T_2\, \mathfrak{g}_{\sigma\tau} = \tau\, \mathfrak{g}_{\sigma\tau}$$

where $\sigma = \pm 1, \tau = \pm 1$. The decomposition and double rotation

$$\begin{aligned} \mathfrak{g} &= \mathfrak{g}_{++} + \mathfrak{g}_{+-} + \mathfrak{g}_{-+} + \mathfrak{g}_{--} \\ &\downarrow T_1 \\ \mathfrak{g}' &= \mathfrak{g}_{++} + \mathfrak{g}_{+-} + \mathrm{i}(\mathfrak{g}_{-+} + \mathfrak{g}_{--}) \\ &\downarrow T_2 \\ \mathfrak{g}'' &= \mathfrak{g}_{++} + i\mathfrak{g}_{+-} + \mathrm{i}(\mathfrak{g}_{-+} + \mathrm{i}\mathfrak{g}_{--}) \end{aligned}$$

generates a noncompact subgroup K'' as well as a pseudo-Riemannian symmetric space P'':

$$K'' = \mathrm{EXP}(\mathfrak{g}_{++} + \mathrm{i}\mathfrak{g}_{+-}), \qquad P'' = \mathrm{EXP}(\mathrm{i}\mathfrak{g}_{-+} + \mathfrak{g}_{--})$$

These have also been classified.

The simplest example of a pseudo-Riemannian symmetric space is SO(2,1)/SO(1,1):

$$\mathfrak{so}(2,1) \to \left[\begin{array}{cc|c} 0 & \theta_3 & \theta_2 \\ -\theta_3 & 0 & \theta_1 \\ \hline \theta_2 & \theta_1 & 0 \end{array}\right] \to \left[\begin{array}{cc|c} 0 & 0 & 0 \\ 0 & 0 & \theta_1 \\ \hline 0 & \theta_1 & 0 \end{array}\right]$$

$$+ \left[\begin{array}{cc|c} 0 & \theta_3 & \theta_2 \\ -\theta_3 & 0 & 0 \\ \hline \theta_2 & 0 & 0 \end{array}\right] \to M = \left[\begin{array}{cc|c} z & x & y \\ -x & * & * \\ \hline y & * & * \end{array}\right]$$

The metric-preserving condition $M^t I_{2,1} M = I_{2,1}$ leads to the constraint equation $z^2 + x^2 - y^2 = 1$. This space is the single-sheeted hyperboloid H_1^2. It is two dimensional and has rank 1, but it is not isotropic. Intersections with the plane $x = 0$ are hyperbolas and with the planes $y = \text{const.}$ are circles. This space is not simply connected.

Summary

Lie groups are among the most powerful mathematical tools available to physicists. They play a major role in physics because they occur as transformation groups from coordinate system to coordinate system in real space (rotation group SO(3), Lorentz group O(3,1), Galilei group, Poincaré group *I*SO(3,1)) or in spaces describing internal degrees of freedom (SU(2) for spin or isospin, SU(3) for quarks and color, SU(4) for spin–isospin, etc.).

It is remarkable that a beautiful classification theory for simple (the building blocks) Lie groups exists, because of the rather amorphous nature of the definition of a Lie group. In a search for structure, the first step in the analysis of Lie groups is linearization of the group multiplication law in the neighborhood of the identity to a linear vector space on which there is a Lie algebra structure. This in itself is sufficient to create a strong connection to quantum mechanics. Although there is not a 1:1 correspondence between Lie groups and their Lie algebras, there is a very beautiful connection between them. This relates algebra (discrete invariant subgroups) and topology (homotopy groups) in an elegant way.

The structure of Lie algebras is described using tools from linear algebra: secular equations and inner products. Together, these tools are used to reduce Lie algebras to their basic units: nilpotent and solvable invariant subalgebras, and semisimple and simple Lie algebras. The commutation relations for simple Lie algebras can be put into a canonical form using another miracle of this theory: a positive-definite root space that summarizes the properties of the secular equation and the Cartan–Killing inner

product. As the secular equation can only be solved exactly over an algebraically closed field, the classification of simple Lie algebras covers complex Lie algebras. Each complex extension has several real forms, which are easily classified.

Even more remarkable is the connection between simple Lie groups and Riemannian spaces that "look the same everywhere." All Riemannian symmetric spaces are quotients of a simple Lie group by a subgroup that is maximal in some precise sense (Cartan decomposition sense). Cartan was able to classify all Riemannian symmetric spaces as a consequence of his classification of all the real forms of all the simple Lie groups. The algebraic tools used to classify Lie algebras (secular equations, Dynkin diagrams) were used again to classify these spaces (Dynkin diagrams → Araki–Satake diagrams). These spaces are classified by a root space, group–subgroup pair, dimension, rank, and character. Construction of invariant operators (Casimir invariants, Laplace–Beltrami operators) is algorithmic.

Nonsemisimple Lie groups/algebras can be constructed from simple Lie algebras by carefully introducing singular change of basis transformations. This leads to "group contraction," not discussed above. In this way, the Poincaré group can be constructed systematically from the groups $SO(3,2)$ or $SO(4,1)$: $SO(3,2) \to ISO(3,1), SO(4,1) \to ISO(3,1)$ in the limit of "large R." Here, R is the "radius" of some universe of hyperbolic nature, with signature $(3,2)$ or $(4,1)$. The Galilei group can be constructed by contraction from the Poincaré group in the limit $c = 3 \times 10^{10}\,\mathrm{cm\,s^{-1}} \to \infty$.

We have not discussed here the theory of the representations of Lie groups. A beautiful theorem by Wigner and Stone guarantees that the tensor representations of a compact group are complete. Gel'fand has given expressions for the complete set of tensor representations of the classical compact Lie groups. They are expressed by "dressing" the appropriate Dynkin diagrams or else in terms of irreducible representations of the symmetric group S_n. Gel'fand has also given explicit, analytic, closed-form expressions for the matrix elements of any of the shift operators in any of these representations. For the noncompact real forms, most of the unitary irreducible representations can be obtained from these expressions for matrix elements ("master analytic representation") by appropriate analytic continuation.

Since Lie groups exist at the interface of algebra and topology, it is to be expected that there is a very close relation with the theory of special functions. In fact, the theory of special functions forms an important chapter in the theory of Lie groups. On the topological side, the shift operators E_α (think $J_\pm$) have coordinate representations $\langle x'|E_\alpha|x\rangle$ involving first-order differential operators. On the algebraic side, the matrix elements $\langle \boldsymbol{n}'|E_\alpha|\boldsymbol{n}\rangle$ are square roots of products of integers (divided by products of integers). These topological and algebraic expressions are related to each other in a myriad of ways. All of the standard properties of special functions (Rodriguez formulas, recursion relations in coordinates and indices, differential equations, generating functions, etc.) occur in a systematic way in a Lie-theoretic formulation of this subject.

Finally, no review or even book could do justice to the applications that Lie group theory finds in physics.

The rich interplay that exists between freedom and rigidity of structure found in Lie group theory can be found in only the purest works of art – for example, the fugues of Bach.

See also: Classical Groups and Homogeneous Spaces; Compact Groups and their Representations; Cosmology: Mathematical Aspects; Equivariant Cohomology and the Cartan Model; Finite-Type Invariants of 3-Manifolds; Functional Equations and Integrable Systems; Lie Superalgebras and Their Representations; Lie, Symplectic, and Poisson Groupoids and Their Lie Algebroids; Measure on Loop Spaces; Quasiperiodic Systems; Symmetry and Symplectic Reduction; Symmetry Classes in Random Matrix Theory; Toda Lattices.

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Lie Superalgebras and Their Representations

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Basic Definitions

Let $\mathcal{A}$ be an algebra over a field $\mathbb{K}$ of characteristic zero (usually $\mathbb{K}=\mathbb{R}$ or $\mathbb{C}$) with internal laws $+$ and $*$. One sets $\mathbb{Z}_2=\mathbb{Z}/2\mathbb{Z}=\{\bar{0},\bar{1}\}$. $\mathcal{A}$ is called a superalgebra or $\mathbb{Z}_2$-graded algebra if it can be written into a direct sum of two spaces $\mathcal{A}=\mathcal{A}_{\bar{0}}\oplus\mathcal{A}_{\bar{1}}$, such that

$$\mathcal{A}_{\bar{0}}*\mathcal{A}_{\bar{0}}\subset\mathcal{A}_{\bar{0}},\quad \mathcal{A}_{\bar{0}}*\mathcal{A}_{\bar{1}}\subset\mathcal{A}_{\bar{1}},\quad \mathcal{A}_{\bar{1}}*\mathcal{A}_{\bar{1}}\subset\mathcal{A}_{\bar{0}}$$

Elements of $\mathcal{A}_{\bar{0}}$ are called even or of degree 0 while elements of $\mathcal{A}_{\bar{1}}$ are called odd or of degree 1. A superalgebra $\mathcal{A}$ is called associative if $(X*Y)*Z=X*(Y*Z)$ for all $X,Y,Z\in\mathcal{A}$. It is called commutative if $X*Y=(-1)^{\deg X.\deg Y}Y*X$ for all $X,Y\in\mathcal{A}$, where $\deg X$ is the degree of the element X.

A homomorphism Φ from a superalgebra $\mathcal{A}$ into a superalgebra $\mathcal{A}'$ is a linear application from $\mathcal{A}$ into $\mathcal{A}'$ which respects the $\mathbb{Z}_2$-gradation, that is, $\Phi(\mathcal{A}_{\bar{0}})\subset\mathcal{A}'_{\bar{0}}$ and $\Phi(\mathcal{A}_{\bar{1}})\subset\mathcal{A}'_{\bar{1}}$.

A Lie superalgebra $\mathcal{G}$ over a field $\mathbb{K}$ of characteristic zero (usually $\mathbb{K}=\mathbb{R}$ or $\mathbb{C}$) is a superalgebra in which the product, denoted $[\![\,,]\!]$, satisfies the following properties:

$\mathbb{Z}_2$-gradation

$$[\![\mathcal{G}_i,\mathcal{G}_j]\!]\subset\mathcal{G}_{i+j}\quad(i,j\in\mathbb{Z}_2)$$

Graded-antisymmetry

$$[\![X_i,X_j]\!]=-(-1)^{\deg X_i.\deg X_j}[\![X_j,X_i]\!]$$

Generalized Jacobi identity

$$\begin{aligned}&(-1)^{\deg X_i.\deg X_k}[\![X_i,[\![X_j,X_k]\!]]\!]\\&+(-1)^{\deg X_j.\deg X_i}[\![X_j,[\![X_k,X_i]\!]]\!]\\&+(-1)^{\deg X_k.\deg X_j}[\![X_k,[\![X_i,X_j]\!]]\!]=0\end{aligned}$$

Note that $\mathcal{G}_{\bar{0}}$ is a Lie algebra, called the even or bosonic part of $\mathcal{G}$, while $\mathcal{G}_{\bar{1}}$, called the odd or fermionic part of $\mathcal{G}$, is not an algebra.

An associative superalgebra $\mathcal{G}=\mathcal{G}_{\bar{0}}\oplus\mathcal{G}_{\bar{1}}$ over the field $\mathbb{K}$ acquires the structure of a Lie superalgebra by taking for the product $[\![\,,]\!]$ of two elements $X,Y\in\mathcal{G}$ the Lie superbracket (also called supercommutator or graded commutator)

$$[\![X,Y]\!]=X*Y-(-1)^{\deg X.\deg Y}Y*X$$

The notation $[\![\,,]\!]$ for the supercommutator is used to avoid confusion with the usual commutator $[X,Y]=X*Y-Y*X$.

A Lie superalgebra $\mathcal{G}$ is $\mathbb{Z}$-graded if it can be written as a direct sum of finite-dimensional $\mathbb{Z}_2$-graded subspaces $\mathcal{G}_i$ such that

$$\mathcal{G}=\bigoplus_{i\in\mathbb{Z}}\mathcal{G}_i,\quad\text{where } [\![\mathcal{G}_i,\mathcal{G}_j]\!]\subset\mathcal{G}_{i+j}$$

The $\mathbb{Z}$-gradation is said to be consistent with the $\mathbb{Z}_2$-gradation if

$$\mathcal{G}_{\bar{0}}=\sum_{i\in\mathbb{Z}}\mathcal{G}_{2i}\quad\text{and}\quad\mathcal{G}_{\bar{1}}=\sum_{i\in\mathbb{Z}}\mathcal{G}_{2i+1}$$

It follows that $\mathcal{G}_0$ is a Lie subalgebra and that each $\mathcal{G}_i(i\neq0)$ is a $\mathcal{G}_0$-module.

A subalgebra $\mathcal{K}=\mathcal{K}_{\bar{0}}\oplus\mathcal{K}_{\bar{1}}$ of a Lie superalgebra $\mathcal{G}$ is a subset of elements of $\mathcal{G}$ which forms a vector subspace of $\mathcal{G}$ that is closed with respect to the Lie product of $\mathcal{G}$ such that $\mathcal{K}_{\bar{0}}\subset\mathcal{G}_{\bar{0}}$ and $\mathcal{K}_{\bar{1}}\subset\mathcal{G}_{\bar{1}}$. A subalgebra $\mathcal{K}$ of $\mathcal{G}$ is called a proper subalgebra of $\mathcal{G}$ if $\mathcal{K}\neq\mathcal{G}$. An ideal $\mathcal{I}$ of $\mathcal{G}$ is a subalgebra of $\mathcal{G}$ such that $[\![\mathcal{G},\mathcal{I}]\!]\subset\mathcal{I}$, that is, $X\in\mathcal{G},Y\in\mathcal{I}\Rightarrow[\![X,Y]\!]\in\mathcal{I}$. An ideal $\mathcal{I}$ of $\mathcal{G}$ is called a proper ideal of $\mathcal{G}$ if $\mathcal{I}\neq\mathcal{G}$. If $\mathcal{I}$ and $\mathcal{I}'$ are two ideals of $\mathcal{G}$, $[\![\mathcal{I},\mathcal{I}']\!]$ is an ideal of $\mathcal{G}$.

The definitions of the centralizer, the center, and the normalizer of a Lie superalgebra follow those of a Lie algebra. Let $\mathcal{S}$ be a subset of elements in the Lie superalgebra $\mathcal{G}$. The centralizer $\mathcal{C}_{\mathcal{G}}(\mathcal{S})$ is the subset of $\mathcal{G}$ given by

$$\mathcal{C}_{\mathcal{G}}(\mathcal{S})=\{X\in\mathcal{G}\,|\,[\![X,Y]\!]=0,\ \forall Y\in\mathcal{S}\}$$

The center $\mathcal{Z}(\mathcal{G})$ of $\mathcal{G}$ is the set of elements of $\mathcal{G}$ which commute with any element of $\mathcal{G}$ (in other words, it is the centralizer of $\mathcal{G}$ in $\mathcal{G}$):

$$\mathcal{Z}(\mathcal{G})=\{X\in\mathcal{G}\,|\,[\![X,Y]\!]=0,\ \forall Y\in\mathcal{G}\}$$

The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{S})$ is the subset of $\mathcal{G}$ given by

$$\mathcal{N}_{\mathcal{G}}(\mathcal{S})=\{X\in\mathcal{G}\,|\,[\![X,Y]\!]\in\mathcal{S},\ \forall Y\in\mathcal{S}\}$$

The Lie superalgebra $\mathcal{G}$ is said to be nilpotent if considering the series $[\![\mathcal{G},\mathcal{G}^{[i-1]}]\!]=\mathcal{G}^{[i]}$ with $\mathcal{G}^{[0]}=\mathcal{G}$, then there exists an integer n such that $\mathcal{G}^{[n]}=\{0\}$.

The Lie superalgebra $\mathcal{G}$ is said to be solvable if considering the series $[\![\mathcal{G}^{(i-1)},\mathcal{G}^{(i-1)}]\!]=\mathcal{G}^{(i)}$ with $\mathcal{G}^{(0)}=\mathcal{G}$, then there exists an integer n such that $\mathcal{G}^{(n)}=\{0\}$. A Lie superalgebra $\mathcal{G}$ is solvable if and only if $\mathcal{G}_{\bar{0}}$ is solvable.

Let $\mathcal{G}$ be a noncommutative Lie superalgebra. The Lie superalgebra $\mathcal{G}$ is called simple if it does not contain any nontrivial ideal. The Lie superalgebra $\mathcal{G}$ is called semisimple if it does not

contain any nontrivial solvable ideal. Let us recall that if $\mathcal{A}$ is a semisimple Lie algebra, it can be written as the direct sum of simple Lie algebras $\mathcal{A}_i : \mathcal{A} = \oplus_i \mathcal{A}_i$. This is not the case for superalgebras.

Let $\mathcal{G} = \mathcal{G}_{\bar{0}} \oplus \mathcal{G}_{\bar{1}}$ be a Lie superalgebra and $\mathcal{V} = \mathcal{V}_{\bar{0}} \oplus \mathcal{V}_{\bar{1}}$ be a $\mathbb{Z}_2$-graded vector space. Consider the algebra End $\mathcal{V}$ of endomorphisms of $\mathcal{V}$, which naturally acquires a superalgebra structure by $\mathrm{End}\,\mathcal{V} = \mathrm{End}_{\bar{0}}\,\mathcal{V} \oplus \mathrm{End}_{\bar{1}}\,\mathcal{V}$, where $\mathrm{End}_i\,\mathcal{V} = \{\phi \in \mathrm{End}\,\mathcal{V} | \phi(\mathcal{V}_j) \subset \mathcal{V}_{i+j}\}$. A linear representation π of $\mathcal{G}$ is a homomorphism of $\mathcal{G}$ into End $\mathcal{V}$, that is,

$$\pi(\alpha X + \beta Y) = \alpha\pi(X) + \beta\pi(Y)$$
$$\pi([\![X, Y]\!]) = [\![\pi(X), \pi(Y)]\!]$$
$$\pi(\mathcal{G}_{\bar{0}}) \subset \mathrm{End}_{\bar{0}}\mathcal{V} \quad \text{and} \quad \pi(\mathcal{G}_{\bar{1}}) \subset \mathrm{End}_{\bar{1}}\mathcal{V}$$

for all $X, Y \in \mathcal{G}$ and $\alpha, \beta \in \mathbb{C}$. The vector space $\mathcal{V}$ is the representation space. The vector space $\mathcal{V}$ has the structure of a $\mathcal{G}$-module by $X(\boldsymbol{v}) = \pi(X)\boldsymbol{v}$ for $X \in \mathcal{G}$ and $\boldsymbol{v} \in \mathcal{V}$. The dimension (resp. superdimension) of the representation π is the dimension (resp. graded dimension) of the vector space $\mathcal{V}$: $\dim \pi = \dim \mathcal{V}_{\bar{0}} + \dim \mathcal{V}_{\bar{1}}$ and $\mathrm{sdim}\pi = \dim \mathcal{V}_{\bar{0}} - \dim \mathcal{V}_{\bar{1}}$. In particular, the representation $\mathrm{ad} : \mathcal{G} \to \mathrm{End}\,\mathcal{G}$ ($\mathcal{G}$ being considered as a $\mathbb{Z}_2$-graded vector space) such that $\mathrm{ad}(X)Y = [\![X, Y]\!]$ is called the adjoint representation of $\mathcal{G}$.

In the basis $(e_1, \ldots, e_m, e_{m+1}, \ldots, e_{m+n})$ of $\mathcal{V} = \mathcal{V}_{\bar{0}} \oplus \mathcal{V}_{\bar{1}}$ (called homogeneous basis), where $\dim \mathcal{V}_{\bar{0}} = m$ and $\dim \mathcal{V}_{\bar{1}} = n$, an element of $\mathcal{G}$ is represented by the matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

where A, B, C, and D are $m \times m, m \times n, n \times m$, and $n \times n$ matrices, respectively. Even elements correspond to block diagonal matrices (i.e., $B = C = 0$), odd elements to block antidiagonal matrices (i.e., $A = D = 0$). One defines the supertrace function denoted by str:

$$\mathrm{str}(M) = \mathrm{tr}(A) - \mathrm{tr}(D)$$

To a given representation π of $\mathcal{G}$, one can associate a bilinear form B_π on $\mathcal{G}$ as

$$B_\pi(X, Y) = \mathrm{str}(\pi(X)\pi(Y)), \quad \forall X, Y \in \mathcal{G}$$

$\pi(X)$ are the matrices of the generators X in the representation π and str denotes the supertrace. A bilinear form B on $\mathcal{G}$ is called

1. consistent if $B(X, Y) = 0$ for all $X \in \mathcal{G}_{\bar{0}}$ and all $Y \in \mathcal{G}_{\bar{1}}$,
2. supersymmetric if, for all $X, Y \in \mathcal{G}$,

$$B(X, Y) = (-1)^{\deg X . \deg Y} B(Y, X)$$

3. invariant if, for all $X, Y, Z \in \mathcal{G}$,

$$B([\![X, Y]\!], Z) = B(X, [\![Y, Z]\!])$$

The bilinear form associated to the adjoint representation of $\mathcal{G}$ is called the Killing form on $\mathcal{G} : K(X, Y) = \mathrm{str}(\mathrm{ad}(X)\mathrm{ad}(Y))$. It is consistent, supersymmetric, and invariant.

Classification of Simple Lie Superalgebras

The simple Lie superalgebras have been classified by V G Kac. One distinguishes two general families: the classical Lie superalgebras and the Cartan type superalgebras.

Classical Lie Superalgebras

A simple Lie superalgebra $\mathcal{G} = \mathcal{G}_{\bar{0}} \oplus \mathcal{G}_{\bar{1}}$ is called classical if the representation of the even subalgebra $\mathcal{G}_{\bar{0}}$ on the odd part $\mathcal{G}_{\bar{1}}$ is completely reducible. The superalgebra is said to be of type I if the representation of $\mathcal{G}_{\bar{0}}$ on $\mathcal{G}_{\bar{1}}$ is the direct sum of two irreducible representations of $\mathcal{G}_{\bar{0}}$. In that case, one has $\mathcal{G}_{\bar{1}} = \mathcal{G}_{-1} \oplus \mathcal{G}_1$ with

$$[\![\mathcal{G}_{-1}, \mathcal{G}_1]\!] = \mathcal{G}_{\bar{0}} \quad \text{and} \quad [\![\mathcal{G}_{\pm 1}, \mathcal{G}_{\pm 1}]\!] = 0$$

The superalgebra is said to be of type II if the representation of $\mathcal{G}_{\bar{0}}$ on $\mathcal{G}_{\bar{1}}$ is irreducible.

A classical Lie superalgebra $\mathcal{G}$ is called basic if there exists a nondegenerate invariant bilinear form on $\mathcal{G}$. The basic Lie superalgebras split into four infinite families: $A(m, n)$ or $\mathrm{sl}(m+1|n+1)$ for $m \neq n$ and $A(n, n)$ or $\mathrm{sl}(n+1|n+1)/\mathcal{Z} = \mathrm{psl}(n+1|n+1)$, where $\mathcal{Z}$ is a one-dimensional center for $m = n$ (unitary series), $B(m, n)$ or $\mathrm{osp}(2m+1|2n)$, $C(n)$ or $\mathrm{osp}(2|2n)$, $D(m, n)$ or $\mathrm{osp}(2m\,|\,2n)$ (orthosymplectic series); and three exceptional superalgebras $F(4)$, $G(3)$, and $D(2, 1; \alpha)$, the last one being actually a one-parameter family of superalgebras. The classical Lie superalgebras which are not basic are called strange, and correspond to two infinite families denoted by $P(n)$ and $Q(n)$.

A basic Lie superalgebra $\mathcal{G} = \mathcal{G}_{\bar{0}} \oplus \mathcal{G}_{\bar{1}}$ admits a consistent $\mathbb{Z}$-gradation $\mathcal{G} = \oplus_{i \in \mathbb{Z}} \mathcal{G}_i$ (called distinguished), such that (see **Tables 1** and **2**)

- for superalgebras of type I, $\mathcal{G}_i = 0$ for $|i| > 1$ and $\mathcal{G}_{\bar{0}} = \mathcal{G}_0, \mathcal{G}_{\bar{1}} = \mathcal{G}_{-1} \oplus \mathcal{G}_1$ and
- for superalgebras of type II, $\mathcal{G}_i = 0$ for $|i| > 2$ and $\mathcal{G}_{\bar{0}} = \mathcal{G}_{-2} \oplus \mathcal{G}_0 \oplus \mathcal{G}_2, \mathcal{G}_{\bar{1}} = \mathcal{G}_{-1} \oplus \mathcal{G}_1$.

Cartan Type Superalgebras

The Cartan type Lie superalgebras are the simple Lie superalgebras in which the representation of the even subalgebra on the odd part is not completely

Table 1 $\mathbb{Z}_2$-gradation of the classical Lie superalgebras

Superalgebra $\mathcal{G}$	$\mathcal{G}_{\bar{0}}$	$\mathcal{G}_{\bar{1}}$
$A(m-1,n-1)$	$A_{m-1} \oplus A_{n-1} \oplus U(1)$	$(m,\bar{n}) \oplus (\bar{m},n)$
$A(n-1,n-1)$	$A_{n-1} \oplus A_{n-1}$	$(n,\bar{n}) \oplus (\bar{n},n)$
$C(n+1)$	$C_n \oplus U(1)$	$(2n) \oplus (2n)$
$B(m,n)$	$B_m \oplus C_n$	$(2m+1,2n)$
$D(m,n)$	$D_m \oplus C_n$	$(2m,2n)$
$F(4)$	$A_1 \oplus B_3$	$(2,8)$
$G(3)$	$A_1 \oplus G_2$	$(2,7)$
$D(2,1;\alpha)$	$A_1 \oplus A_1 \oplus A_1$	$(2,2,2)$
$P(n)$	A_n	$[2] \oplus [1^{n-1}]$
$Q(n)$	A_n	$\mathrm{ad}(A_n)$

reducible. They are classified into four infinite families called $W(n)$ with $n \geq 2, S(n)$ with $n \geq 3$, $\widetilde{S}(n)$, and $H(n)$ with $n \geq 4$. $S(n)$ and $\widetilde{S}(n)$ are called special Cartan type Lie superalgebras and $H(n)$ Hamiltonian Cartan type Lie superalgebras.

Classical Lie Superalgebras

The classical Lie superalgebras are described as matrix superalgebras as follows. Let $\mathcal{V} = \mathcal{V}_{\bar{0}} \oplus \mathcal{V}_{\bar{1}}$ be a $\mathbb{Z}_2$-graded vector space, with $\dim \mathcal{V}_{\bar{0}} = m$, $\dim \mathcal{V}_{\bar{1}} = n$. The Lie superalgebra $\mathrm{gl}(m|n)$ is defined as the superalgebra $\mathrm{End}\,\mathcal{V} = \mathrm{End}_{\bar{0}}\,\mathcal{V} \oplus \mathrm{End}_{\bar{1}}\,\mathcal{V}$ supplied with the Lie superbracket.

The unitary superalgebra $A(m-1,n-1) = \mathrm{sl}(m\,|\,n)$ is defined as the superalgebra of matrices $M \in \mathrm{gl}(m|n)$ satisfying the supertrace condition $\mathrm{str}(M) = 0$. In the case $m = n, \mathrm{sl}(n|n)$ contains a one-dimensional ideal $\mathcal{I}$ generated by $\mathbb{I}_{2n}$ and one sets $A(n-1,n-1) = \mathrm{sl}(n\,|\,n)/\mathcal{I} \equiv \mathrm{psl}(n\,|\,n)$.

The orthosymplectic superalgebra $\mathrm{osp}(m\,|\,2n)$ is defined as the superalgebra of matrices $M \in \mathrm{gl}(m\,|\,n)$ satisfying the conditions

$$A^{\mathrm{t}} = -A, \quad D^{\mathrm{t}}G = -GD, \quad B = C^{\mathrm{t}}G$$

where t denotes the usual transposition and the matrix G is given by

$$G = \begin{pmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{pmatrix}$$

The strange superalgebra $P(n)$ is defined as the superalgebra of matrices $M \in \mathrm{gl}(n\,|\,n)$ satisfying the conditions

$$A^{\mathrm{t}} = -D, \quad B^{\mathrm{t}} = B, \quad C^{\mathrm{t}} = -C, \quad \mathrm{tr}(A) = 0$$

The strange superalgebra $\widetilde{Q}(n)$ is defined as the superalgebra of matrices $M \in \mathrm{gl}(n\,|\,n)$ satisfying the conditions

$$A = D, \quad B = C, \quad \mathrm{tr}(B) = 0$$

The superalgebra $\widetilde{Q}(n)$ has a one-dimensional center $\mathcal{Z}$. The simple superalgebra $Q(n)$ is given by $Q(n) = \widetilde{Q}(n)/\mathcal{Z}$.

Structure of the Classical Lie Superalgebras

Let $\mathcal{G} = \mathcal{G}_{\bar{0}} \oplus \mathcal{G}_{\bar{1}}$ be a classical Lie superalgebra. A Cartan subalgebra $\mathcal{H}$ of $\mathcal{G}$ is defined as a Cartan subalgebra of $\mathcal{G}_{\bar{0}}$, that is, the maximal nilpotent subalgebra of $\mathcal{G}_{\bar{0}}$ coinciding with its own normalizer: $\mathcal{H} = \{X \in \mathcal{G}_{\bar{0}} \,|\, [\![X,\mathcal{H}]\!] \subseteq \mathcal{H}\}$. It follows that the Cartan subalgebras of a Lie superalgebra are conjugate since the Cartan subalgebras of a Lie algebra are conjugate and any inner automorphism of the even part $\mathcal{G}_{\bar{0}}$ can be extended to an inner automorphism of $\mathcal{G}$; hence, they all have the same dimension. By definition, the dimension of a Cartan subalgebra $\mathcal{H}$ is the rank of $\mathcal{G}$: $\mathrm{rank}\,\mathcal{G} = \dim \mathcal{H}$.

A classical Lie superalgebra $\mathcal{G}$ with Cartan subalgebra $\mathcal{H}$ can be decomposed as $\mathcal{G} = \bigoplus_{\alpha \in \mathcal{H}^*} \mathcal{G}_\alpha$ ($\mathcal{H}^*$ is the dual of $\mathcal{H}$), where

$$\mathcal{G}_\alpha = \{x \in \mathcal{G} \,|\, [\![h,x]\!] = \alpha(h)x, h \in \mathcal{H}\}$$

The set $\Delta \subset \mathcal{H}^*$

$$\Delta = \{\alpha \in \mathcal{H}^* | \mathcal{G}_\alpha \neq 0\}$$

is by definition the root system of $\mathcal{G}$. A root α is called even (resp. odd) if $\mathcal{G}_\alpha \cap \mathcal{G}_{\bar{0}} \neq \emptyset$ (resp.

Table 2 $\mathbb{Z}$-gradation of the classical basic Lie superalgebras

Superalgebra $\mathcal{G}$	$\mathcal{G}_0$	$\mathcal{G}_1 \oplus \mathcal{G}_{-1}$	$\mathcal{G}_2 \oplus \mathcal{G}_{-2}$
$A(m-1,n-1)$	$A_{m-1} \oplus A_{n-1} \oplus U(1)$	$(m,\bar{n}) \oplus (\bar{m},n)$	
$A(n-1,n-1)$	$A_{n-1} \oplus A_{n-1}$	$(n,\bar{n}) \oplus (\bar{n},n)$	
$C(n+1)$	$C_n \oplus U(1)$	$(2n)_+ \oplus (2n)_-$	
$B(m,n)$	$B_m \oplus A_{n-1} \oplus U(1)$	$(2m+1,n) \oplus (2m+1,\bar{n})$	$[2] \oplus [2^{n-1}]$
$D(m,n)$	$D_m \oplus A_{n-1} \oplus U(1)$	$(2m,n) \oplus (2m,\bar{n})$	$[2] \oplus [2^{n-1}]$
$F(4)$	$B_3 \oplus U(1)$	$8_+ \oplus 8_-$	$1_+ \oplus 1_-$
$G(3)$	$G_2 \oplus U(1)$	$7_+ \oplus 7_-$	$1_+ \oplus 1_-$
$D(2,1;\alpha)$	$A_1 \oplus A_1 \oplus U(1)$	$(2,2)_+ \oplus (2,2)_-$	$1_+ \oplus 1_-$

$\mathcal{G}_\alpha \cap \mathcal{G}_{\bar{1}} \neq \emptyset$). The set of even roots $\Delta_{\bar{0}}$ is the root system of the even part $\mathcal{G}_{\bar{0}}$ of $\mathcal{G}$. The set of odd root $\Delta_{\bar{1}}$ is the weight system of the representation of $\mathcal{G}_{\bar{0}}$ in $\mathcal{G}_{\bar{1}}$. One has $\Delta = \Delta_{\bar{0}} \cup \Delta_{\bar{1}}$. A root can be both even and odd (however this only occurs in the case of the superalgebra $Q(n)$). The vector space spanned by all the possible roots is called the root space. It is the dual $\mathcal{H}^*$ of the Cartan subalgebra $\mathcal{H}$ as vector space.

Except for $A(1,1), P(n)$, and $Q(n)$, using a nondegenerate invariant bilinear form B on the superalgebra $\mathcal{G}$, one can define a bilinear form $(\cdot,\cdot)$ on the root space $\mathcal{H}^*$ by $(\alpha_i, \alpha_j) = B(H_i, H_j)$, where the H_i form a basis of $\mathcal{H}$. The following properties hold:

1. $\mathcal{G}_{(\alpha=0)} = \mathcal{H}$ except for $Q(n)$.
2. $\dim \mathcal{G}_\alpha = 1$ when $\alpha \neq 0$ except for $A(1,1), P(2)$, $P(3)$, and $Q(n)$.
3. Except for $A(1,1), P(n), Q(n)$, one has
   (a) $[\![\mathcal{G}_\alpha, \mathcal{G}_\beta]\!] \neq 0$ if and only if $\alpha, \beta, \alpha+\beta \in \Delta$,
   (b) $(\mathcal{G}_\alpha, \mathcal{G}_\beta) = 0$ for $\alpha + \beta \neq 0$,
   (c) if $\alpha \in \Delta$ (resp. $\Delta_{\bar{0}}, \Delta_{\bar{1}}$), then $-\alpha \in \Delta$ (resp. $\Delta_{\bar{0}}, \Delta_{\bar{1}}$), and
   (d) $\alpha \in \Delta \Rightarrow 2\alpha \in \Delta$ if and only if $\alpha \in \Delta_{\bar{1}}$ and $(\alpha,\alpha) \neq 0$.

In the rest of this section, we restrict to the case of a basic Lie superalgebra $\mathcal{G}$ of rank r, with Cartan subalgebra $\mathcal{H}$ and root system $\Delta = \Delta_{\bar{0}} \cup \Delta_{\bar{1}}$. Then $\mathcal{G}$ admits a Borel decomposition $\mathcal{G} = \mathcal{N}^+ \oplus \mathcal{H} \oplus \mathcal{N}^-$, where $\mathcal{N}^\pm$ are subalgebras such that $[\mathcal{H}, \mathcal{N}^\pm] \subset \mathcal{N}^\pm$ with $\dim \mathcal{N}^+ = \dim \mathcal{N}^-$. If $\mathcal{G} = \mathcal{H} \bigoplus_\alpha \mathcal{G}_\alpha$ is the root decomposition of $\mathcal{G}$, a root α is called positive if $\mathcal{G}_\alpha \cap \mathcal{N}^+ \neq \emptyset$ and negative if $\mathcal{G}_\alpha \cap \mathcal{N}^- \neq \emptyset$. A root is called simple if it cannot be decomposed into a sum of positive roots. The set of all simple roots is called a simple root system of $\mathcal{G}$ and is denoted here by Δ^0. The set $\mathcal{B} = \mathcal{H} \oplus \mathcal{N}^+$ is called a Borel subalgebra of $\mathcal{G}$. Such a Borel subalgebra is solvable but not maximal solvable. Indeed, adding to $\mathcal{B}$ a negative simple isotropic root generator (i.e., a generator associated to an odd root of zero length), the obtained subalgebra is still solvable since the superalgebra sl(1|1) is solvable. However, $\mathcal{B}$ contains a maximal solvable subalgebra $\mathcal{B}_{\bar{0}}$ of the even part $\mathcal{G}_{\bar{0}}$.

In general, for a basic Lie superalgebra $\mathcal{G}$, there are many inequivalent classes of conjugacy of Borel subalgebras (while for the simple Lie algebras, all Borel subalgebras are conjugate).

To each class of conjugacy of Borel subalgebras of $\mathcal{G}$ is associated a simple root system Δ^0. Hence, contrary to the Lie algebra case, to a given basic Lie superalgebra $\mathcal{G}$ will be associated in general many inequivalent simple root systems, up to a transformation of the Weyl group $W(\mathcal{G})$ of $\mathcal{G}$ (the Weyl group of a basic Lie superalgebra being generated by the Weyl reflections with respect to the even roots; under a transformation of $W(\mathcal{G})$, a simple root system will be transformed into an equivalent one with the same Dynkin diagram). The generalization of the Weyl group for a basic Lie superalgebra $\mathcal{G}$ gives a method for constructing all the simple root systems of $\mathcal{G}$ and hence all the inequivalent Dynkin diagrams of $\mathcal{G}$. For $\alpha \in \Delta_{\bar{1}}$, one defines

$$
\begin{aligned}
w_\alpha(\beta) &= \beta - 2\frac{(\alpha,\beta)}{(\alpha,\alpha)}\alpha \quad \text{if } (\alpha,\alpha) \neq 0 \\
w_\alpha(\beta) &= \beta + \alpha \quad \text{if } (\alpha,\alpha) = 0,\ (\alpha,\beta) \neq 0 \\
w_\alpha(\beta) &= \beta \quad \text{if } (\alpha,\alpha) = (\alpha,\beta) = 0 \\
w_\alpha(\alpha) &= -\alpha
\end{aligned}
$$

Note that the transformation associated to an odd root α of zero length cannot be lifted to an automorphism of the superalgebra since w_α transforms even roots into odd ones, and vice versa, and the $\mathbb{Z}_2$-gradation would not be respected. A simple root system Δ^0 being given, from any root $\alpha \in \Delta^0$ such that $(\alpha,\alpha) = 0$, one constructs the simple root system $w_\alpha(\Delta^0)$, where w_α is the generalized Weyl reflection with respect to α and one repeats the procedure on the obtained system until no new basis arises.

In the set of all inequivalent simple root systems of a basic Lie superalgebra, there is one simple root system that plays a particular role, the distinguished simple root system, for which the number of odd roots is equal to one, constructed as follows. Consider the distinguished $\mathbb{Z}$-gradation of $\mathcal{G}, \mathcal{G} = \oplus_{i \in \mathbb{Z}} \mathcal{G}_i$. The even simple roots are given by the simple root system of the Lie subalgebra $\mathcal{G}_0$ and the odd simple root is the lowest weight of the representation $\mathcal{G}_1$ of $\mathcal{G}_0$. See **Table 3** for the root systems and **Table 4** for the distinguished simple root systems of the basic Lie superalgebras.

Let $\Delta^0 = (\alpha_1, \ldots, \alpha_r)$ be a simple root system of $\mathcal{G}$, such that $(\alpha_i, \alpha_j) \in \mathbb{Z}$ and $|\min(\alpha_i, \alpha_j)| = 1$ if $(\alpha_i, \alpha_j) \neq 0$. Then one defines the symmetric Cartan matrix a with integer entries as $a_{ij} = (\alpha_i, \alpha_j)$. One associates to Δ^0 a Dynkin diagram according to the following rules:

1. One associates to each simple even root a white dot, to each simple odd root of nonzero length ($a_{ii} \neq 0$) a black dot, and to each simple odd root of zero length ($a_{ii} = 0$) a gray dot.

Table 3 Root systems $\Delta_{\bar{0}}, \Delta_{\bar{1}}$ of the basic Lie superalgebras

Superalgebra $\mathcal{G}$	$\Delta_{\bar{0}}$	$\Delta_{\bar{1}}$
$A(m-1, n-1)$	$\varepsilon_i - \varepsilon_j, \delta_k - \delta_l$	$\pm(\varepsilon_i - \delta_k)$
$B(m,n)$	$\pm\varepsilon_i \pm \varepsilon_j,\ \pm\varepsilon_i,\ \pm\delta_k \pm \delta_l,\ \pm 2\delta_k$	$\pm\varepsilon_i \pm \delta_k,\ \pm\delta_k$
$B(0, n)$	$\pm\delta_k \pm \delta_l,\ \pm 2\delta_k$	$\pm\delta_k$
$C(n+1)$	$\pm\delta_k \pm \delta_l,\ \pm 2\delta_k$	$\pm\varepsilon \pm \delta_k$
$D(m,n)$	$\pm\varepsilon_i \pm \varepsilon_j,\ \pm\delta_k \pm \delta_l,\ \pm 2\delta_k$	$\pm\varepsilon_i \pm \delta_k$
$F(4)$	$\pm\delta,\ \pm\varepsilon_i \pm \varepsilon_j,\ \pm\varepsilon_i$	$\frac{1}{2}(\pm\varepsilon_1 \pm \varepsilon_2 \pm \varepsilon_3 \pm \delta)$
$G(3)$	$\pm 2\delta,\ \pm\varepsilon_i, \varepsilon_i - \varepsilon_j$	$\pm\delta,\ \pm\varepsilon_i \pm \delta$
$D(2,1;\alpha)$	$\pm 2\varepsilon_i$	$\pm\varepsilon_1 \pm \varepsilon_2 \pm \varepsilon_3$

$1 \le i,j \le m, 1 \le k,l \le n$ for $A(m-1,n-1), B(m,n), C(n+1), D(m,n)$. $1 \le i,j \le 3$ for $F(4), G(3), D(2,1;\alpha)$, with $\varepsilon_1 + \varepsilon_2 + \varepsilon_3 = 0$ in the case of $G(3)$. For $A(n-1,n-1)$, one has to add the condition $\varepsilon_1 + \cdots + \varepsilon_n = \delta_1 + \cdots + \delta_n$.

Table 4 Distinguished simple root systems of the basic Lie superalgebras

Superalgebra $\mathcal{G}$	Distinguished simple root system Δ^0
$A(m-1, n-1)$	$\delta_1 - \delta_2, \ldots, \delta_{n-1} - \delta_n, \delta_n - \varepsilon_1, \varepsilon_1 - \varepsilon_2, \ldots, \varepsilon_{m-1} - \varepsilon_m$
$B(m, n)$	$\delta_1 - \delta_2, \ldots, \delta_{n-1} - \delta_n, \delta_n - \varepsilon_1, \varepsilon_1 - \varepsilon_2, \ldots, \varepsilon_{m-1} - \varepsilon_m, \varepsilon_m$
$B(0, n)$	$\delta_1 - \delta_2, \ldots, \delta_{n-1} - \delta_n, \delta_n$
$C(n)$	$\varepsilon - \delta_1, \delta_1 - \delta_2, \ldots, \delta_{n-1} - \delta_n, 2\delta_n$
$D(m, n)$	$\delta_1 - \delta_2, \ldots, \delta_{n-1} - \delta_n, \delta_n - \varepsilon_1, \varepsilon_1 - \varepsilon_2, \ldots, \varepsilon_{m-1} - \varepsilon_m, \varepsilon_{m-1} + \varepsilon_m$
$F(4)$	$\frac{1}{2}(\delta - \varepsilon_1 - \varepsilon_2 - \varepsilon_3), \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2$
$G(3)$	$\delta + \varepsilon_3, \varepsilon_1, \varepsilon_2 - \varepsilon_1$
$D(2,1;\alpha)$	$\varepsilon_1 - \varepsilon_2 - \varepsilon_3, 2\varepsilon_2, 2\varepsilon_3$

2. The ith and jth dots are joined by η_{ij} lines where

$$\eta_{ij} = \frac{2|a_{ij}|}{\min(|a_{ii}|, |a_{jj}|)} \qquad \text{if } a_{ii}.a_{jj} \neq 0$$
$$\eta_{ij} = \frac{2|a_{ij}|}{\min(|a_{ii}|, 2)} \qquad \text{if } a_{ii} \neq 0 \text{ and } a_{jj} = 0$$
$$\eta_{ij} = |a_{ij}| \qquad \text{if } a_{ii} = a_{jj} = 0$$

3. We add an arrow on the lines connecting the ith and jth dots when $\eta_{ij} > 1$, pointing from i to j if $a_{ii}.a_{jj} \neq 0$ and $|a_{ii}| > |a_{jj}|$ or if $a_{ii} = 0, a_{jj} \neq 0$, $|a_{jj}| < 2$, and pointing from j to i if $a_{ii} = 0$, $a_{jj} \neq 0, |a_{jj}| > 2$.
4. For $D(2,1;\alpha), \eta_{ij} = 1$ if $a_{ij} \neq 0$ and $\eta_{ij} = 0$ if $a_{ij} = 0$. No arrow is put on the Dynkin diagram.

The distinguished Dynkin diagrams of the basic Lie superalgebras are listed in **Table 5**.

Representation Theory of Basic Lie Superalgebras

We restrict in the following to the basic Lie superalgebras. We assume that $\mathcal{G} \neq \mathrm{psl}(n,n)$ but the following results still hold for $\mathrm{sl}(n\,|\,n)$. Let $\mathcal{G} = \mathcal{N}^+ \oplus \mathcal{H} \oplus \mathcal{N}^-$ be a Borel decomposition of $\mathcal{G}$ where $\mathcal{N}^+$ (resp. $\mathcal{N}^-$) is spanned by the positive (resp. negative) root generators of $\mathcal{G}, \mathcal{H}$ is a Cartan subalgebra, and $\mathcal{H}^*$ is the dual of $\mathcal{H}$. A representation $\pi: \mathcal{G} \to \mathrm{End}\,\mathcal{V}$ with representation space $\mathcal{V}$ is called a highest-weight representation with highest weight $\Lambda \in \mathcal{H}^*$ if there exists a nonzero vector $v_\Lambda \in \mathcal{V}$ such that

$$\mathcal{N}^+ v_\Lambda = 0$$
$$h(v_\Lambda) = \Lambda(h) v_\Lambda (h \in \mathcal{H})$$

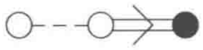
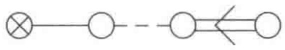
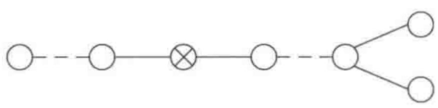
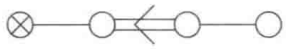
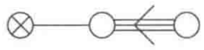
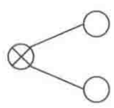
The $\mathcal{G}$-module $\mathcal{V}$ is called a highest-weight module, denoted by $\mathcal{V}(\Lambda)$, and the vector $v_\Lambda \in \mathcal{V}$ a highest-weight vector. From now on, $\mathcal{H}$ is the distinguished Cartan subalgebra of $\mathcal{G}$ with basis of generators $(H_1, \ldots, H_r)$ where $r = \mathrm{rank}\,\mathcal{G}$ and H_s denotes the Cartan generator associated to the odd simple root. The Kac–Dynkin labels are defined by

$$a_i = 2\frac{(\Lambda, \alpha_i)}{(\alpha_i, \alpha_i)} \quad \text{for} \quad i \neq s \quad \text{and} \quad a_s = (\Lambda, \alpha_s)$$

A weight $\Lambda \in \mathcal{H}^*$ is called a dominant weight if $a_i \ge 0$ for all $i \neq s$, integral if $a_i \in \mathbb{Z}$ for all $i \neq s$, and integral dominant if $a_i \in \mathbb{Z}_{\ge 0}$ for all $i \neq s$. A necessary condition for the highest-weight representation of $\mathcal{G}$ with highest weight Λ to be finite dimensional is that Λ be an integral dominant weight.

One then defines the Kac module. Consider $\mathcal{G} = \oplus_{i\in\mathbb{Z}} \mathcal{G}_i$ the distinguished $\mathbb{Z}$-gradation of $\mathcal{G}$ and let $\mathcal{K} = \mathcal{G}_0 \oplus \mathcal{N}^+$, where $\mathcal{N}^+ = \oplus_{i>0} \mathcal{G}_i$, be a subalgebra of $\mathcal{G}$. Denote by $\mathcal{U}(\mathcal{G})$ and $\mathcal{U}(\mathcal{K})$ the corresponding universal enveloping superalgebras. Let $\Lambda \in \mathcal{H}^*$ be an integral dominant weight and $\mathcal{V}_0(\Lambda)$ be the $\mathcal{G}_0$-module with highest weight Λ, which is extended to a $\mathcal{K}$-module by setting

Table 5 Distinguished Dynkin diagrams of the basic Lie superalgebras

Superalgebra $\mathcal{G}$	*Distinguished Dynkin diagram*
$A(m-1, n-1)$	
$B(m, n)$	
$B(0, n)$	
$C(n+1)$	
$D(m, n)$	
$F(4)$	
$G(3)$	
$D(2, 1; \alpha)$	

$\mathcal{N}^+\mathcal{V}_0(\Lambda) = 0$. From this $\mathcal{K}$-module, it is possible to construct a $\mathcal{G}$-module in the following way. One considers the factor space $\mathcal{U}(\mathcal{G}) \otimes_{\mathcal{U}(\mathcal{K})} \mathcal{V}_0(\Lambda)$ consisting of elements of $\mathcal{U}(\mathcal{G}) \otimes \mathcal{V}_0(\Lambda)$ such that the elements $h \otimes \boldsymbol{v}$ and $1 \otimes h(\boldsymbol{v})$ have been identified for $h \in \mathcal{K}$ and $\boldsymbol{v} \in \mathcal{V}_0(\Lambda)$. This space acquires the structure of a $\mathcal{G}$-module by setting $g(\boldsymbol{u} \otimes \boldsymbol{v}) = g\boldsymbol{u} \otimes \boldsymbol{v}$ for $\boldsymbol{u} \in \mathcal{U}(\mathcal{G}), g \in \mathcal{G}$, and $\boldsymbol{v} \in \mathcal{V}_0(\Lambda)$. This $\mathcal{G}$-module is called the induced module from the $\mathcal{K}$-module $\mathcal{V}_0(\Lambda)$ and denoted by $\mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\mathcal{V}_0(\Lambda)$. For example, in the case of type I basic Lie superalgebras, if $\{f_1, \ldots, f_d\}$ denotes a basis of odd generators of $\mathcal{G}/\mathcal{K}$, then

$$\mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\mathcal{V}_0(\Lambda) = \bigoplus_{1 \le i_1 < \cdots < i_k \le d} f_{i_1} \ldots f_{i_k} \mathcal{V}_0(\Lambda)$$

The Kac module $\overline{\mathcal{V}}(\Lambda)$ is defined as follows:

1. For a superalgebra $\mathcal{G}$ of type I (the odd part is the direct sum of two irreducible representations of the even part), the Kac module is the induced module

$$\overline{\mathcal{V}}(\Lambda) = \mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\ \mathcal{V}_0(\Lambda)$$

2. For a superalgebra $\mathcal{G}$ of type II (the odd part is an irreducible representation of the even part), the induced module $\mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\ \mathcal{V}_0(\Lambda)$ contains a submodule $\mathcal{M}(\Lambda) = \mathcal{U}(\mathcal{G})\mathcal{G}_{-\psi}^{b+1}\mathcal{V}_0(\Lambda)$, where ψ is the longest simple root of $\mathcal{G}_{\bar{0}}$ which is hidden behind the odd simple root – that is, the longest simple root of $\mathrm{sp}(2n)$ in the case of $\mathrm{osp}(m\,|\,2n)$ and the simple root of $\mathrm{sl}(2)$ in the case of $F(4), G(3)$, and $D(2, 1; \alpha)$ – and $b = 2(\Lambda, \psi)/(\psi, \psi)$ is the component of Λ with respect to ψ. The Kac module is defined as the quotient of the induced module $\mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\ \mathcal{V}_0(\Lambda)$ by the submodule $\mathcal{M}(\Lambda)$:

$$\overline{\mathcal{V}}(\Lambda) = \mathrm{Ind}_{\mathcal{K}}^{\mathcal{G}}\ \mathcal{V}_0(\Lambda)/\mathcal{U}(\mathcal{G})\mathcal{G}_{-\psi}^{b+1}\mathcal{V}_0(\Lambda)$$

In the case where the Kac module is not simple, it contains a maximal submodule $\mathcal{I}(\Lambda)$ and the quotient module $\mathcal{V}(\Lambda) = \overline{\mathcal{V}}(\Lambda)/\mathcal{I}(\Lambda)$ is a simple module.

The fundamental result concerning the representations of basic Lie superalgebras is the following:

1. Any finite dimensional irreducible representation of $\mathcal{G}$ is of the form $\mathcal{V}(\Lambda) = \overline{\mathcal{V}}(\Lambda)/\mathcal{I}(\Lambda)$, where Λ is an integral dominant weight.
2. Any finite-dimensional simple $\mathcal{G}$-module is uniquely characterized by its integral dominant weight Λ: two $\mathcal{G}$-modules $\mathcal{V}(\Lambda)$ and $\mathcal{V}(\Lambda')$ are isomorphic if and only if $\Lambda = \Lambda'$.
3. The finite-dimensional simple $\mathcal{G}$-module $\mathcal{V}(\Lambda) = \overline{\mathcal{V}}(\Lambda)/\mathcal{I}(\Lambda)$ has the weight decomposition

$$\mathcal{V}(\Lambda) = \bigoplus_{\lambda \le \Lambda} \mathcal{V}_\lambda$$

with

$$\mathcal{V}_\lambda = \{\boldsymbol{v} \in \mathcal{V} | h(\boldsymbol{v}) = \lambda(h)\boldsymbol{v}, h \in \mathcal{H}\}$$

The presence of odd roots will have another important consequence in the representation theory of superalgebras. Indeed, one might find that in certain representations, weight vectors, different from the highest one specifying the representation, are annihilated by all the generators corresponding to positive roots. Such vector have, of course, to be decoupled from the representation. Representations of this kind are called atypical, while the other irreducible representations not suffering this pathology are called typical. For a basic Lie superalgebra $\mathcal{G}$ with root system Δ, one defines $\overline{\Delta}_{\bar{0}} = \{\alpha \in \Delta_{\bar{0}} | \alpha/2 \notin \Delta_{\bar{1}}\}$ and $\overline{\Delta}_{\bar{1}} = \{\alpha \in \Delta_{\bar{1}} | 2\alpha \notin \Delta_{\bar{0}}\}$. Let ρ_0 be the half-sum of the roots of $\Delta_{\bar{0}}^+$, ρ_1 the half-sum of the roots of $\Delta_{\bar{1}}^+$, and $\rho = \rho_0 - \rho_1$. The representation π with highest weight Λ is called typical if

$$(\Lambda + \rho, \alpha) \neq 0 \quad \text{for all } \alpha \in \overline{\Delta}_{\bar{1}}^+$$

The highest weight Λ is then called typical. If there exists some $\alpha \in \overline{\Delta}_{\bar{1}}^+$ such that $(\Lambda + \rho, \alpha) = 0$,

the representation π and the highest weight Λ are called atypical. The number of distinct elements $\alpha \in \overline{\Delta}_{\bar{1}}^{+}$ for which Λ is atypical is the degree of atypicality of the representation π. If there exists one and only one $\alpha \in \overline{\Delta}_{\bar{1}}^{+}$ such that $(\Lambda + \rho, \alpha) = 0$, the representation π and the highest weight Λ are called singly atypical.

The Kac module $\overline{\mathcal{V}}(\Lambda)$ is a simple $\mathcal{G}$-module if and only if the highest weight Λ is typical. All the finite-dimensional representations of $B(0,n)$ are typical. All the finite-dimensional representations of $C(n+1)$ are either typical or singly atypical.

The dimension of a typical finite-dimensional representation $\mathcal{V}$ of $\mathcal{G}$ is given by

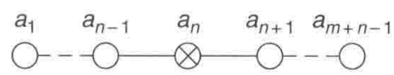
$$\dim \mathcal{V}(\Lambda) = 2^{\dim \Delta_{\bar{1}}^{+}} \prod_{\alpha \in \Delta_{\bar{0}}^{+}} \frac{(\Lambda + \rho, \alpha)}{(\rho_0, \alpha)}$$

where $\dim \mathcal{V}_{\bar{0}}(\Lambda) = \dim \mathcal{V}_{\bar{1}}(\Lambda)$ if $\mathcal{G} \neq B(0,n)$, and if $\mathcal{G} = B(0,n)$,

$$\dim \mathcal{V}_{\bar{0}}(\Lambda) - \dim \mathcal{V}_{\bar{1}}(\Lambda) = \prod_{\alpha \in \overline{\Delta}_{\bar{0}}^{+}} \frac{(\Lambda + \rho, \alpha)}{(\overline{\rho}_0, \alpha)}$$

The atypicality conditions are the following:

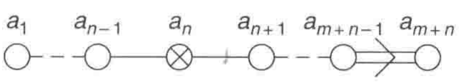
- For $A(m,n)$ with $\Lambda = (a_1, \ldots, a_{m+n-1})$



$$\sum_{k=i}^{n-1} a_k - \sum_{k=n+1}^{j} a_k + a_n = i + j - 2n$$

where $1 \le i \le n \le j \le m+n-1$.

- $B(m,n)$ with $\Lambda = (a_1, \ldots, a_{m+n})(m \neq 0)$

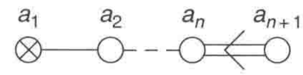


$$\sum_{q=i}^{n} a_q - \sum_{q=n+1}^{j} a_q = i + j - 2n$$

$$\sum_{q=i}^{n} a_q - \sum_{q=n+1}^{j} a_q - 2\sum_{q=j+1}^{m+n-1} a_q - a_{m+n} = 2m + i - j - 1 = 0$$

where $1 \le i \le n \le j \le m+n-1$.

- $C(n+1)$ with $\Lambda = (a_1, \ldots, a_{n+1})$

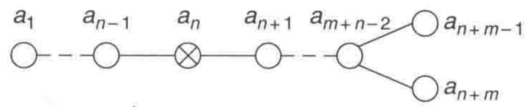


$$a_1 - \sum_{q=2}^{i} a_q - i + 1 = 0$$

$$a_1 - \sum_{q=2}^{i} a_q - 2\sum_{q=i+1}^{n+1} a_q - 2n + i - 1 = 0$$

where $1 \le i \le n$.

- $D(m \mid n)$ with $\Lambda = (a_1, \ldots, a_{m+n})$



$$\sum_{q=i}^{n} a_q - \sum_{q=n+1}^{j} a_q = i + j - 2n$$

where $1 \le i \le n \le j \le m+n-1$

$$\sum_{q=i}^{n} a_q - \sum_{q=n+1}^{m+n-2} a_q - a_{m+n} = m - n + i - 1$$

where $1 \le i \le n$

$$\sum_{q=i}^{n} a_q - \sum_{q=n+1}^{j} a_q - 2\sum_{q=j+1}^{m+n-2} a_q = a_{m+n-1} + a_{m+n} + 2m + i - j - 2$$

where $1 \le i \le n \le j \le m+n-2$

See also: Lie Groups: General Theory; Lie, Symplectic, and Poisson Groupoids and Their Lie Algebroids.

Further Reading

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Lie, Symplectic, and Poisson Groupoids and Their Lie Algebroids

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Introduction

Groupoids are mathematical structures able to describe symmetry properties more general than those described by groups. They were introduced (and named) by H Brandt in 1926. Around 1950, Charles Ehresmann used groupoids with additional structures (topological and differentiable) as essential tools in topology and differential geometry. In recent years, Mickael Karasev, Alan Weinstein, and Stanisław Zakrzewski independently discovered that symplectic groupoids can be used for the construction of noncommutative deformations of the algebra of smooth functions on a manifold, with potential applications to quantization. Poisson groupoids were introduced by Alan Weinstein as generalizations of both Poisson Lie groups and symplectic groupoids.

We present here the main definitions and first properties relative to groupoids, Lie groupoids, Lie algebroids, symplectic and Poisson groupoids and their Lie algebroids.

Groupoids

What is a Groupoid?

Before stating the formal definition of a groupoid, let us explain, in an informal way, why it is a very natural concept. The easiest way to understand that concept is to think of two sets, Γ and Γ_0. The first one, Γ, is called the "set of arrows" or "total space" of the groupoid, and the other one, Γ_0, the "set of objects" or "set of units" of the groupoid. One may consider an element $x \in \Gamma$ as an arrow going from an object (a point in Γ_0) to another object (another point in Γ_0). The word "arrow" is used here in a very general sense: it means a way for going from a point in Γ_0 to another in Γ_0. One should not consider an arrow as a line drawn in the set Γ_0 joining the starting point of the arrow to its endpoint: this happens only for some special groupoids. Rather, one should think of an arrow as living outside Γ_0, with only its starting point and its endpoint in Γ_0, as shown in **Figure 1**.

The following ingredients enter the definition of a groupoid.

1. Two maps $\alpha : \Gamma \to \Gamma_0$ and $\beta : \Gamma \to \Gamma_0$, called the "target map" and the "source map" of the groupoid. If $x \in \Gamma$ is an arrow, $\alpha(x) \in \Gamma_0$ is its endpoint and $\beta(x) \in \Gamma_0$ its starting point.
2. A "composition law" on the set of arrows; we can compose an arrow y with another arrow x, and get an arrow $m(x,y)$, by following first the arrow y, then the arrow x. Of course, $m(x,y)$ is defined if and only if the target of y is equal to the source of x. The source of $m(x,y)$ is equal to the source of y, and its target is equal to the target of x, as illustrated in **Figure 1**. It is only by convention that we write $m(x,y)$ rather than $m(y,x)$: the arrow which is followed first is on the right, by analogy with the usual notation $f \circ g$ for the composition of two maps g and f. When there is no risk of confusion, we write $x \circ y$, or $x \,.\, y$, or even simply xy for $m(x,y)$. The composition of arrows is associative.
3. An "embedding" ε of the set Γ_0 into the set Γ, which associates a unit arrow $\varepsilon(u)$ with each $u \in \Gamma_0$. That unit arrow is such that both its source and its target are u, and it plays the role of a unit when composed with another arrow, either on the right or on the left: for any arrow x, $m(\varepsilon(\alpha(x)), x) = x$, and $m(x, \varepsilon(\beta(x))) = x$.
4. Finally, an "inverse map" ι from the set of arrows onto itself. If $x \in \Gamma$ is an arrow, one may think of $\iota(x)$ as the arrow x followed in the reverse sense. We often write x^{-1} for $\iota(x)$.

Now we are ready to state the formal definition of a groupoid.

Definition 1 A groupoid is a pair of sets (Γ, Γ_0) equipped with the structure defined by the following data:

(i) an injective map $\varepsilon : \Gamma_0 \to \Gamma$, called the unit section of the groupoid;

(ii) two maps $\alpha : \Gamma \to \Gamma_0$ and $\beta : \Gamma \to \Gamma_0$, called, respectively, the target map and the source map; they satisfy

$$\alpha \circ \varepsilon = \beta \circ \varepsilon = \mathrm{id}_{\Gamma_0} \qquad [1]$$

(iii) a composition law $m : \Gamma_2 \to \Gamma$, called the product, defined on the subset Γ_2 of $\Gamma \times \Gamma$, called the set of composable elements,

$$\Gamma_2 = \{(x,y) \in \Gamma \times \Gamma;\ \beta(x) = \alpha(y)\} \qquad [2]$$

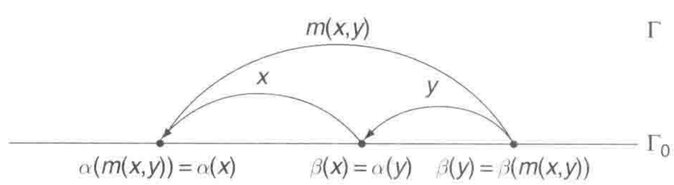


Figure 1 Two arrows x and $y \in \Gamma$, with the target of y, $\alpha(y) \in \Gamma_0$, equal to the source of x, $\beta(x) \in \Gamma_0$, and the composed arrow $m(x,y)$.

which is associative, in the sense that whenever one side of the equality

$$m(x, m(y, z)) = m(m(x, y), z) \qquad [3]$$

is defined, the other side is defined too, and the equality holds; moreover, the composition law m is such that for each $x \in \Gamma$,

$$m(\varepsilon(\alpha(x)), x) = m(x, \varepsilon(\beta(x))) = x \qquad [4]$$

(iv) a map $\iota : \Gamma \to \Gamma$, called the inverse, such that, for every $x \in \Gamma$, $(x, \iota(x)) \in \Gamma_2$ and $(\iota(x), x) \in \Gamma_2$, and

$$m(x, \iota(x)) = \varepsilon(\alpha(x)), \quad m(\iota(x), x) = \varepsilon(\beta(x)) \qquad [5]$$

The sets Γ and Γ_0 are called, respectively, the total space and the set of units of the groupoid, which is itself denoted by $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$.

Identification and Notations

In what follows, by means of the injective map ε, we will identify the set of units Γ_0 with the subset $\varepsilon(\Gamma_0)$ of Γ. Therefore, ε will be the canonical injection in Γ of its subset Γ_0.

For x and $y \in \Gamma$, we will sometimes write $x \,.\, y$, or even simply xy for $m(x, y)$, and x^{-1} for $\iota(x)$. In addition, we will write "the groupoid Γ" for "the groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$."

Properties and Comments

The above definitions have the following consequences.

Involutivity of the inverse map The inverse map ι is involutive:

$$\iota \circ \iota = \mathrm{id}_\Gamma \qquad [6]$$

We have indeed, for any $x \in \Gamma$,

$$\begin{aligned} \iota \circ \iota(x) &= m(\iota \circ \iota(x), \beta(\iota \circ \iota(x))) \\ &= m(\iota \circ \iota(x), \beta(x)) = m(\iota \circ \iota(x), m(\iota(x), x)) \\ &= m(m(\iota \circ \iota(x), \iota(x)), x) = m(\alpha(x), x) = x \end{aligned}$$

Unicity of the inverse Let x and $y \in \Gamma$ be such that

$$m(x, y) = \alpha(x) \quad \text{and} \quad m(y, x) = \beta(x)$$

Then we have

$$\begin{aligned} y &= m(y, \beta(y)) = m(y, \alpha(x)) \\ &= m(y, m(x, \iota(x))) = m(m(y, x), \iota(x)) \\ &= m(\beta(x), \iota(x)) = m(\alpha(\iota(x)), \iota(x)) = \iota(x) \end{aligned}$$

Therefore for any $x \in \Gamma$, the unique $y \in \Gamma$ such that $m(y, x) = \beta(x)$ and $m(x, y) = \alpha(x)$ is $\iota(x)$.

The fibers of α and β and the isotropy groups The target map α (resp. the source map β) of a groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ determines an equivalence relation on Γ: two elements x and $y \in \Gamma$ are said to be α-equivalent (resp. β-equivalent) if $\alpha(x) = \alpha(y)$ (resp. if $\beta(x) = \beta(y)$). The corresponding equivalence classes are called the α-fibers (resp. the β-fibers) of the groupoid. They are of the form $\alpha^{-1}(u)$ (resp. $\beta^{-1}(u)$), with $u \in \Gamma_0$.

For each unit $u \in \Gamma_0$, the subset

$$\begin{aligned} \Gamma_u &= \alpha^{-1}(u) \cap \beta^{-1}(u) \\ &= \{x \in \Gamma;\ \alpha(x) = \beta(x) = u\} \end{aligned} \qquad [7]$$

is called the "isotropy group" of u. It is indeed a group, with the restrictions of m and ι as composition law and inverse map.

A way to visualize groupoids We have seen (**Figure 1**) a way in which groupoids may be visualized, by using arrows for elements in Γ and points for elements in Γ_0. There is another very useful way to visualize groupoids, shown in **Figure 2**.

The total space Γ of the groupoid is represented as a plane, and the set Γ_0 of units as a straight line in that plane. The α-fibers (resp. the β-fibers) are represented as parallel straight lines, transverse to Γ_0.

Examples of Groupoids

The groupoid of pairs Let E be a set. The "groupoid of pairs" of elements in E has, as its total space, the product space $E \times E$. The diagonal $\Delta_E = \{(x, x); x \in E\}$ is its set of units, and the target and source maps are

$$\alpha : (x, y) \mapsto (x, x), \qquad \beta : (x, y) \mapsto (y, y)$$

Its composition law m and inverse map ι are

$$\begin{aligned} m((x, y), (y, z)) &= (x, z) \\ \iota((x, y)) &= (x, y)^{-1} = (y, x) \end{aligned}$$

Groups A group G is a groupoid with set of units $\{e\}$, with only one element e, the unit element of the

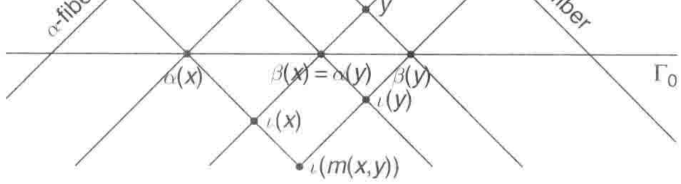


Figure 2 A way to visualize groupoids.

group. The target and source maps are both equal to the constant map $x \mapsto e$.

Definition 2 A topological groupoid is a groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ for which Γ is a (maybe non-Hausdorff) topological space, Γ_0 a Hausdorff topological subspace of Γ, α and β surjective continuous maps, $m:\Gamma_2 \to \Gamma$ a continuous map, and $\iota:\Gamma \to \Gamma$ a homeomorphism.

A Lie groupoid is a groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ for which Γ is a smooth (maybe non-Hausdorff) manifold, Γ_0 a smooth Hausdorff submanifold of Γ, α and β smooth surjective submersions (which implies that Γ_2 is a smooth submanifold of $\Gamma \times \Gamma$), $m:\Gamma_2 \to \Gamma$ a smooth map, and $\iota:\Gamma \to \Gamma$ a smooth diffeomorphism.

Properties of Lie Groupoids

Dimensions Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a Lie groupoid. Since α and β are submersions, for any $x \in \Gamma$, the α-fiber $\alpha^{-1}(\alpha(x))$ and the β-fiber $\beta^{-1}(\beta(x))$ are submanifolds of Γ, both of dimension $\dim \Gamma - \dim \Gamma_0$. The inverse map ι, restricted to the α-fiber through x (resp. the β-fiber through x), is a diffeomorphism of that fiber onto the β-fiber through $\iota(x)$ (resp. the α-fiber through $\iota(x)$). The dimension of the submanifold Γ_2 of composable pairs in $\Gamma \times \Gamma$ is $2\dim \Gamma - \dim \Gamma_0$.

The tangent bundle of a Lie groupoid Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a Lie groupoid. Its tangent bundle $T\Gamma$ is a Lie groupoid, with $T\Gamma_0$ as set of units, $T\alpha: T\Gamma \to T\Gamma_0$ and $T\beta: T\Gamma \to T\Gamma_0$ as target and source maps. Let us denote by Γ_2 the set of composable pairs in $\Gamma \times \Gamma$, by $m:\Gamma_2 \to \Gamma$ the composition law, and by $\iota:\Gamma \to \Gamma$ the inverse. Then the set of composable pairs in $T\Gamma \times T\Gamma$ is simply $T\Gamma_2$, the composition law on $T\Gamma$ is $Tm: T\Gamma_2 \to T\Gamma$, and the inverse is $T\iota: T\Gamma \to T\Gamma$.

When the groupoid Γ is a Lie group G, the Lie groupoid TG is a Lie group too. We will see that the cotangent bundle of a Lie groupoid is a Lie groupoid, and more precisely a symplectic groupoid.

Isotropy groups For each unit $u \in \Gamma_0$ of a Lie groupoid, the isotropy group Γ_u (defined earlier) is a Lie group.

Examples of Topological and Lie Groupoids

Topological groups and Lie groups A topological group (resp. a Lie group) is a topological groupoid (resp. a Lie groupoid) whose set of units has only one element e.

Vector bundles A smooth vector bundle $\pi: E \to M$ on a smooth manifold M is a Lie groupoid, with the base M as set of units (identified with the image of the zero section); the source and target maps both coincide with the projection π; the product and the inverse maps are the addition $(x, y) \mapsto x + y$ and the opposite map $x \mapsto -x$ in the fibers.

The fundamental groupoid of a topological space Let M be a topological space. A "path" in M is a continuous map $\gamma:[0,1] \to M$. We denote by $[\gamma]$ the homotopy class of a path γ and by $\Pi(M)$ the set of homotopy classes of paths in M (with fixed end-points). For $[\gamma] \in \Pi(M)$, we set $\alpha([\gamma]) = \gamma(1)$, $\beta([\gamma]) = \gamma(0)$, where γ is any representative of the class $[\gamma]$. The concatenation of paths determines a well-defined composition law on $\Pi(M)$, for which $\Pi(M) \overset{\alpha}{\underset{\beta}{\rightrightarrows}} M$ is a topological groupoid, called the "fundamental groupoid" of M. The inverse map is $[\gamma] \mapsto [\gamma^{-1}]$, where γ is any representative of $[\gamma]$ and γ^{-1} is the path $t \mapsto \gamma(1-t)$. The set of units is M, if we identify a point in M with the homotopy class of the constant path equal to that point.

When M is a smooth manifold, the same construction can be made with piecewise smooth paths, and the fundamental groupoid $\Pi(M) \overset{\alpha}{\underset{\beta}{\rightrightarrows}} M$ is a Lie groupoid.

Symplectic and Poisson Groupoids

Symplectic and Poisson Geometry

Let us recall some definitions and results in symplectic and Poisson geometry, used in the next sections.

Symplectic manifolds A "symplectic form" on a smooth manifold M is a differential 2-form ω, which is closed, that is, which satisfies

$$d\omega = 0 \qquad [8]$$

and nondegenerate, that is, such that for each point $x \in M$ and each nonzero vector $v \in T_xM$, there exists a vector $w \in T_xM$ such that $\omega(v, w) \neq 0$. Equipped with the symplectic form ω, a smooth manifold M is called a "symplectic manifold" and denoted by (M, ω).

The dimension of a symplectic manifold is always even.

The Liouville form on a cotangent bundle Let N be a smooth manifold, and T^*N be its cotangent bundle. The Liouville form on T^*N is the 1-form θ such that, for any $\eta \in T^*N$ and $v \in T_\eta(T^*N)$,

$$\theta(v) = \langle \eta, T\pi_N(v) \rangle \qquad [9]$$

where $\pi_N: T^*N \to N$ is the canonical projection.

The 2-form $\omega = d\theta$ is symplectic, and is called the "canonical symplectic form" on the cotangent bundle T^*N.

Poisson manifolds A Poisson manifold is a smooth manifold P equipped with a bivector field (i.e., a smooth section of $\wedge^2 TP$) Π which satisfies

$$[\Pi, \Pi] = 0 \qquad [10]$$

the bracket on the left-hand side being the Schouten bracket. The bivector field Π will be called the Poisson structure on P. It allows us to define a composition law on the space $C^\infty(P, \mathbb{R})$ of smooth functions on P, called the Poisson bracket and denoted by $(f,g) \mapsto \{f,g\}$, by setting, for all f and $g \in C^\infty(P, \mathbb{R})$ and $x \in P$,

$$\{f,g\}(x) = \Pi(\mathrm{d}f(x), \mathrm{d}g(x)) \qquad [11]$$

That composition law is skew-symmetric and satisfies the Jacobi identity, therefore turns $C^\infty(P, \mathbb{R})$ into a Lie algebra.

Hamiltonian vector fields Let (P, Π) be a Poisson manifold. We denote by $\Pi^\sharp : T^*P \to TP$ the vector bundle map defined by

$$\langle \eta, \Pi^\sharp(\zeta) \rangle = \Pi(\zeta, \eta) \qquad [12]$$

where ζ and η are two elements in the same fiber of T^*P. Let $f : P \to \mathbb{R}$ be a smooth function on P. The vector field $X_f = \Pi^\sharp(\mathrm{d}f)$ is called the Hamiltonian vector field associated to f. If $g : P \to \mathbb{R}$ is another smooth function on P, the Poisson bracket $\{f,g\}$ can be written as

$$\{f,g\} = \langle \mathrm{d}g, \Pi^\sharp(\mathrm{d}f) \rangle = -\langle \mathrm{d}f, \Pi^\sharp(\mathrm{d}g) \rangle \qquad [13]$$

The canonical Poisson structure on a symplectic manifold Every symplectic manifold (M, ω) has a Poisson structure, associated to its symplectic structure, for which the vector bundle map $\Pi^\sharp : T^*M \to M$ is the inverse of the vector bundle isomorphism $v \mapsto -\mathrm{i}(v)\omega$. We will always consider that a symplectic manifold is equipped with that Poisson structure, unless otherwise specified.

The KKS Poisson structure Let $\mathcal{G}$ be a finite-dimensional Lie algebra. Its dual space $\mathcal{G}^*$ has a natural Poisson structure, for which the bracket of two smooth functions f and g is

$$\{f,g\}(\xi) = \langle \xi, [\mathrm{d}f(\xi), \mathrm{d}g(\xi)] \rangle \qquad [14]$$

with $\xi \in \mathcal{G}^*$, the differentials $\mathrm{d}f(\xi)$ and $\mathrm{d}g(\xi)$ being considered as elements in $\mathcal{G}$, identified with its bidual $\mathcal{G}^{**}$. It is called the Kirillov, Kostant, and Souriau (KKS) Poisson structure on $\mathcal{G}^*$.

Poisson maps Let (P_1, Π_1) and (P_2, Π_2) be two Poisson manifolds. A smooth map $\varphi : P_1 \to P_2$ is called a Poisson map if, for every pair (f,g) of smooth functions on P_2,

$$\{\varphi^* f, \varphi^* g\}_1 = \varphi^* \{f,g\}_2 \qquad [15]$$

Product Poisson structures The product $P_1 \times P_2$ of two Poisson manifolds (P_1, Π_1) and (P_2, Π_2) has a natural Poisson structure: it is the unique Poisson structure for which the bracket of functions of the form $(x_1, x_2) \mapsto f_1(x_1) f_2(x_2)$ and $(x_1, x_2) \mapsto g_1(x_1) g_2(x_2)$ (where f_1 and $g_1 \in C^\infty(P_1, \mathbb{R})$, f_2 and $g_2 \in C^\infty(P_2, \mathbb{R})$) is

$$(x_1, x_2) \mapsto \{f_1, g_1\}_1(x_1) \{f_2, g_2\}_2(x_2)$$

The same property holds for the product of any finite number of Poisson manifolds.

Symplectic orthogonality Let (V, ω) be a symplectic vector space, that means a real, finite-dimensional vector space V with a skew-symmetric nondegenerate bilinear form ω. Let W be a vector subspace of V. The "symplectic orthogonal" of W is

$$\operatorname{orth} W = \{v \in V; \omega(v, w) = 0 \text{ for all } w \in W\} \qquad [16]$$

It is a vector subspace of V, which satisfies

$$\dim W + \dim(\operatorname{orth} W) = \dim V, \qquad \operatorname{orth}(\operatorname{orth} W) = W$$

The vector subspace W is said to be isotropic if $W \subset \operatorname{orth} W$, coisotropic if $\operatorname{orth} W \subset W$, and Lagrangian if $W = \operatorname{orth} W$. In any symplectic vector space, there are many Lagrangian subspaces; therefore, the dimension of a symplectic vector space is always even; if $\dim V = 2n$, the dimension of an isotropic (resp. coisotropic, resp. Lagrangian) vector subspace is $\leq n$ (resp. $\geq n$, resp. $= n$).

Coisotropic and Lagrangian submanifolds A submanifold N of a Poisson manifold (P, Π) is said to be coisotropic if the bracket of two smooth functions, defined on an open subset of P and which vanish on N, vanishes on N too. A submanifold N of a symplectic manifold (M, ω) is coisotropic if and only if for each point $x \in N$, the vector subspace T_xN of the symplectic vector space $(T_xM, \omega(x))$ is coisotropic. Therefore, the dimension of a coisotropic submanifold in a $2n$-dimensional symplectic manifold is $\geq n$; when it is equal to n, the submanifold N is said to be Lagrangian.

Poisson quotients Let $\varphi : M \to P$ be a surjective submersion of a symplectic manifold (M, ω) onto a

manifold P. The manifold P has a Poisson structure Π for which φ is a Poisson map if and only if $\text{orth}(\ker T\varphi)$ is integrable. When that condition is satisfied, that Poisson structure on P is unique.

Poisson Lie groups A Poisson Lie group is a Lie group G with a Poisson structure Π, such that the product $(x,y) \mapsto xy$ is a Poisson map from $G \times G$, endowed with the product Poisson structure, into (G, Π). The Poisson structure of a Poisson Lie group (G, Π) always vanishes at the unit element e of G. Therefore, the Poisson structure of a Poisson Lie group never comes from a symplectic structure on that group.

Definition 3 A symplectic groupoid (resp. a Poisson groupoid) is a Lie groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ with a symplectic form ω on Γ (resp. with a Poisson structure Π on Γ) such that the graph of the composition law m

$$\{(x,y,z) \in \Gamma \times \Gamma \times \Gamma; (x,y) \in \Gamma_2 \text{ and } z = m(x,y)\}$$

is a Lagrangian submanifold (resp. a coisotropic submanifold) of $\Gamma \times \Gamma \times \bar{\Gamma}$ with the product symplectic form (resp. the product Poisson structure), the first two factors Γ being endowed with the symplectic form ω (resp. with the Poisson structure Π), and the third factor $\bar{\Gamma}$ being Γ with the symplectic form $-\omega$ (resp. with the Poisson structure $-\Pi$).

The next theorem states important properties of symplectic and Poisson groupoids.

Theorem 4 *Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a symplectic groupoid with symplectic 2-form ω (resp. a Poisson groupoid with Poisson structure Π). We have the following properties.*

(i) *For a symplectic groupoid, given any point $c \in \Gamma$, each one of the two vector subspaces of the symplectic vector space $(T_c\Gamma, \omega(c))$,*

$$T_c(\beta^{-1}(\beta(c))) \quad \text{and} \quad T_c(\alpha^{-1}(\alpha(c)))$$

is the symplectic orthogonal of the other one. For a symplectic or Poisson groupoid, if f is a smooth function whose restriction to each α-fiber is constant, and g a smooth function whose restriction to each β-fiber is constant, then the Poisson bracket $\{f,g\}$ vanishes identically.

(ii) *The submanifold of units Γ_0 is a Lagrangian submanifold of the symplectic manifold (Γ, ω) (resp. a coisotropic submanifold of the Poisson manifold (Γ, Π)).*

(iii) *The inverse map $\iota : \Gamma \to \Gamma$ is an antisymplectomorphism of (Γ, ω), that is, it satisfies $\iota^*\omega = -\omega$ (resp. an anti-Poisson diffeomorphism of (Γ, Π), i.e., it satisfies $\iota_*\Pi = -\Pi$).*

Corollary 5 *Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a symplectic groupoid with symplectic 2-form ω (resp. a Poisson groupoid with Poisson structure Π). There exists on Γ_0 a unique Poisson structure Π_0 for which $\alpha : \Gamma \to \Gamma_0$ is a Poisson map, and $\beta : \Gamma \to \Gamma_0$ an anti-Poisson map (i.e., β is a Poisson map when Γ_0 is equipped with the Poisson structure $-\Pi_0$).*

Examples of Symplectic and Poisson Groupoids

The cotangent bundle of a Lie groupoid Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a Lie groupoid.

We have seen above that its tangent bundle $T\Gamma$ has a Lie groupoid structure, determined by that of Γ. Similarly (but much less obviously), the cotangent bundle $T^*\Gamma$ has a Lie groupoid structure determined by that of Γ. The set of units is the conormal bundle to the submanifold Γ_0 of Γ, denoted by $\mathcal{N}^*\Gamma_0$. We recall that $\mathcal{N}^*\Gamma_0$ is the vector sub-bundle of $T^*_{\Gamma_0}\Gamma$ (the restriction to Γ_0 of the cotangent bundle $T^*\Gamma$), whose fiber $\mathcal{N}^*_p\Gamma_0$ at a point $p \in \Gamma_0$ is

$$\mathcal{N}^*_p\Gamma_0 = \left\{\eta \in T^*_p\Gamma; \langle \eta, v\rangle = 0 \text{ for all } v \in T_p\Gamma_0\right\}$$

To define the target and source maps of the Lie algebroid $T^*\Gamma$, we introduce the notion of "bisection" through a point $x \in \Gamma$. A bisection through x is a submanifold A of Γ, with $x \in A$, transverse both to the α-fibers and to the β-fibers, such that the maps α and β, when restricted to A, are diffeomorphisms of A onto open subsets $\alpha(A)$ and $\beta(A)$ of Γ_0, respectively. For any point $x \in M$, there exist bisections through x. A bisection A allows us to define two smooth diffeomorphisms between open subsets of Γ, denoted by L_A and R_A and called the left and right translations by A, respectively. They are defined by

$$L_A : \alpha^{-1}(\beta(A)) \to \alpha^{-1}(\alpha(A))$$
$$L_A(y) = m\left(\beta|_A^{-1} \circ \alpha(y), y\right)$$

and

$$R_A : \beta^{-1}(\alpha(A)) \to \beta^{-1}(\beta(A))$$
$$R_A(y) = m\left(y, \alpha|_A^{-1} \circ \beta(y)\right)$$

The definitions of the target and source maps for $T^*\Gamma$ rest on the following properties. Let x be a point in Γ and A be a bisection through x. The two vector subspaces, $T_{\alpha(x)}\Gamma_0$ and $\ker T_{\alpha(x)}\beta$, are complementary in $T_{\alpha(x)}\Gamma$. For any $v \in T_{\alpha(x)}\Gamma, v - T\beta(v)$ is in $\ker T_{\alpha(x)}\beta$. Moreover, R_A maps the fiber

$\beta^{-1}(\alpha(x))$ into the fiber $\beta^{-1}(\beta(x))$, and its restriction to that fiber does not depend on the choice of A; it depends only on x. Therefore, $TR_A(v - T\beta(v))$ is in ker $T_x\beta$ and does not depend on the choice of A. We can define the map $\widehat{\alpha}$ by setting, for any $\xi \in T_x^*\Gamma$ and any $v \in T_{\alpha(x)}\Gamma$,

$$\langle \widehat{\alpha}(\xi), v \rangle = \langle \xi, TR_A(v - T\beta(v)) \rangle$$

Similarly, we define $\widehat{\beta}$ by setting, for any $\xi \in T_x^*\Gamma$ and any $w \in T_{\beta(x)}\Gamma$,

$$\left\langle \widehat{\beta}(\xi), w \right\rangle = \langle \xi, TL_A(w - T\alpha(w)) \rangle$$

We see that $\widehat{\alpha}$ and $\widehat{\beta}$ are unambiguously defined, smooth, and take their values in the submanifold $\mathcal{N}^*\Gamma_0$ of $T^*\Gamma$. They satisfy

$$\pi_\Gamma \circ \widehat{\alpha} = \alpha \circ \pi_\Gamma, \qquad \pi_\Gamma \circ \widehat{\beta} = \beta \circ \pi_\Gamma$$

where $\pi_\Gamma : T^*\Gamma \to \Gamma$ is the cotangent bundle projection.

Let us now define the composition law $\widehat{m}$ on $T^*\Gamma$. Let $\xi \in T_x^*\Gamma$ and $\eta \in T_y^*\Gamma$ be such that $\widehat{\beta}(\xi) = \widehat{\alpha}(\eta)$. This implies $\beta(x) = \alpha(y)$. Let A be a bisection through x and B a bisection through y. There exist a unique $\xi_{b\alpha} \in T_{\alpha(x)}^*\Gamma_0$ and a unique $\eta_{b\beta} \in T_{\beta(y)}^*\Gamma_0$ such that

$$\xi = (L_A^{-1})^*\left(\widehat{\beta}(\xi)\right) + \alpha_x^*\xi_{b\alpha}$$
$$\eta = (R_B^{-1})^*(\widehat{\alpha}(\xi)) + \beta_y^*\eta_{b\beta}$$

Then $\widehat{m}(\xi, \eta)$ is given by

$$\widehat{m}(\xi, \eta) = \alpha_{xy}^*\xi_{b\alpha} + \beta_{xy}^*\eta_{b\beta} + (R_B^{-1})^*(L_A^{-1})^*\left(\widehat{\beta}(x)\right)$$

We observe that in the last term of the above expression we can replace $\widehat{\beta}(\xi)$ by $\widehat{\alpha}(\eta)$, since these two expressions are equal, and that $(R_B^{-1})^*(L_A^{-1})^* = (L_A^{-1})^*(R_B^{-1})^*$, since R_B and L_A commute.

Finally, the inverse $\widehat{\iota}$ in $T^*\Gamma$ is ι^*.

With its canonical symplectic form, $T^*\Gamma \overset{\widehat{\alpha}}{\underset{\widehat{\beta}}{\rightrightarrows}} \mathcal{N}^*\Gamma_0$ is a symplectic groupoid. When the Lie groupoid Γ is a Lie group G, the Lie groupoid T^*G is not a Lie group, contrary to what happens for TG. This shows that the introduction of Lie groupoids is not at all artificial: when dealing with Lie groups, Lie groupoids are already with us! The set of units of the Lie groupoid T^*G can be identified with $\mathcal{G}^*$ (the dual of the Lie algebra $\mathcal{G}$ of G), identified itself with T_e^*G (the cotangent space to G at the unit element e). The target map $\widehat{\alpha} : T^*G \to T_e^*G$ (resp. the source map $\widehat{\beta} : T^*G \to T_e^*G$) associates to each $g \in G$ and $\xi \in T_g^*G$, the value at the unit element e of the right-invariant 1-form (resp. the left-invariant 1-form) whose value at x is ξ.

Poisson Lie groups as Poisson groupoids Poisson groupoids were introduced by Alan Weinstein as a generalization of both symplectic groupoids and Poisson Lie groups. Indeed, a Poisson Lie group is a Poisson groupoid with a set of units reduced to a single element.

Lie Algebroids

The notion of a Lie algebroid, due to Jean Pradines, is related to that of a Lie groupoid in the same way as the notion of a Lie algebra is related to that of a Lie group.

Definition 6 A Lie algebroid over a smooth manifold M is a smooth vector bundle $\pi : A \to M$ with base M, equipped with

(i) a composition law $(s_1, s_2) \mapsto \{s_1, s_2\}$ on the space $\Gamma^\infty(\pi)$ of smooth sections of π, called the bracket, for which that space is a Lie algebra; and
(ii) a vector bundle map $\rho : A \to TM$, over the identity map of M, called the anchor map, such that, for all s_1 and $s_2 \in \Gamma^\infty(\pi)$ and all $f \in C^\infty(M, \mathbb{R})$,

$$\{s_1, fs_2\} = f\{s_1, s_2\} + ((\rho \circ s_1) \cdot f)s_2 \qquad [17]$$

Examples

Lie algebras A finite-dimensional Lie algebra is a Lie algebroid (with a base reduced to a point and the zero map as anchor map).

Tangent bundles and their integrable sub-bundles A tangent bundle $\tau_M : TM \to M$ to a smooth manifold M is a Lie algebroid, with the usual bracket of vector fields on M as composition law, and the identity map as anchor map. More generally, any integrable vector sub-bundle F of a tangent bundle $\tau_M : TM \to M$ is a Lie algebroid, still with the bracket of vector fields on M with values in F as composition law and the canonical injection of F into TM as anchor map.

The cotangent bundle of a Poisson manifold Let (P, Π) be a Poisson manifold. Its cotangent bundle $\pi_P : T^*P \to P$ has a Lie algebroid structure, with $\Pi^\sharp : T^*P \to TP$ as anchor map. The composition law is the bracket of 1-forms. It will be denoted by $(\eta, \zeta) \mapsto [\eta, \zeta]$ (in order to avoid any confusion with the Poisson bracket of functions). It is given by the formula, in which η and ζ are 1-forms and X a vector field on P:

$$\langle [\eta, \zeta], X \rangle = \Pi(\eta, d\langle \zeta, X \rangle) + \Pi(d\langle \eta, X \rangle, \zeta) + (\mathcal{L}(X)\Pi)(\eta, \zeta) \qquad [18]$$

We have denoted by $\mathcal{L}(X)\Pi$ the Lie derivative of the Poisson structure Π with respect to the vector

field X. Another equivalent formula for that composition law is

$$[\zeta, \eta] = \mathcal{L}(\Pi^\sharp \zeta)\eta - \mathcal{L}(\Pi^\sharp \eta)\zeta - \mathrm{d}(\Pi(\zeta, \eta)) \quad [19]$$

The bracket of 1-forms is related to the Poisson bracket of functions by

$$[\mathrm{d}f, \mathrm{d}g] = \mathrm{d}\{f, g\} \quad \text{for all } f \text{ and } g \in C^\infty(P, \mathbb{R}) \quad [20]$$

Properties of Lie Algebroids

Let $\pi : A$ be a Lie algebroid with anchor map $\rho : A \to TM$.

A Lie algebras homomorphism For any pair (s_1, s_2) of smooth sections of π,

$$\rho \circ \{s_1, s_2\} = [\rho \circ s_1, \rho \circ s_2]$$

which means that the map $s \mapsto \rho \circ s$ is a Lie algebra homomorphism from the Lie algebra of smooth sections of π into the Lie algebra of smooth vector fields on M.

The generalized Schouten bracket The composition law $(s_1, s_2) \mapsto \{s_1, s_2\}$ on the space of sections of π extends into a composition law on the space of sections of exterior powers of (A, π, M), which is called the “generalized Schouten bracket.” Its properties are the same as those of the usual Schouten bracket. When the Lie algebroid is a tangent bundle $\tau_M : TM \to M$, that composition law reduces to the usual Schouten bracket. When the Lie algebroid is the cotangent bundle $\pi_P : T^*P \to P$ to a Poisson manifold (P, Π), the generalized Schouten bracket is the bracket of forms of all degrees on the Poisson manifold P, introduced by J-L Koszul, which extends the bracket of 1-forms used earlier.

The dual bundle of a Lie algebroid Let $\varpi : A^* \to M$ be the dual bundle of the Lie algebroid $\pi : A \to M$. There exists on the space of sections of its exterior powers a graded endomorphism d_ρ, of degree 1 (that means that if η is a section of $\wedge^k A^*$, $d_\rho(\eta)$ is a section of $\wedge^{k+1} A^*$). That endomorphism satisfies

$$d_\rho \circ d_\rho = 0$$

and its properties are essentially the same as those of the exterior derivative of differential forms. When the Lie algebroid is a tangent bundle $\tau_M : TM \to M$, d_ρ is the usual exterior derivative of differential forms.

On the spaces of sections of the exterior powers of a Lie algebroid and of its dual bundle we can develop a differential calculus very similar to the usual differential calculus of vector and multivector fields and differential forms on a manifold. Operators such as the interior product, the exterior derivative, and the Lie derivative can still be defined and have properties similar to those of the corresponding operators for vector and multivector fields and differential forms on a manifold.

The total space A^* of the dual bundle of a Lie algebroid $\pi : A \to M$ has a natural Poisson structure: a smooth section s of π can be considered as a smooth real-valued function on A^* whose restriction to each fiber $\varpi^{-1}(x) (x \in M)$ is linear; this property allows us to extend the bracket of sections of π (defined by the Lie algebroid structure) to obtain a Poisson bracket of functions on A^*. When the Lie algebroid A is a finite-dimensional Lie algebra $\mathcal{G}$, the Poisson structure on its dual space $\mathcal{G}^*$ is the KKS Poisson structure discussed earlier.

The Lie Algebroid of a Lie Groupoid

Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a Lie groupoid. Let $A(\Gamma)$ be the intersection of $\ker T\alpha$ and $T_{\Gamma_0}\Gamma$ (the tangent bundle $T\Gamma$ restricted to the submanifold Γ_0). We see that $A(\Gamma)$ is the total space of a vector bundle $\pi : A(\Gamma) \to \Gamma_0$, with base Γ_0, the canonical projection π being the map which associates a point $u \in \Gamma_0$ to every vector in $\ker T_u\alpha$. In this section, we define a composition law on the set of smooth sections of that bundle, and a vector bundle map $\rho : A(\Gamma) \to T\Gamma_0$, for which $\pi : A(\Gamma) \to \Gamma_0$ is a Lie algebroid, called the Lie algebroid of the Lie groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$.

We observe first that for any point $u \in \Gamma_0$ and any point $x \in \beta^{-1}(u)$, the map $L_x : y \mapsto L_x y = m(x, y)$ is defined on the α-fiber $\alpha^{-1}(u)$, and maps that fiber into the α-fiber $\alpha^{-1}(\alpha(x))$. Therefore, $T_u L_x$ maps the vector space $A_u = \ker T_u\alpha$ onto the vector space $\ker T_x\alpha$, tangent at x to the α-fiber $\alpha^{-1}(\alpha(x))$. Any vector $w \in A_u$ can therefore be extended into the vector field along $\beta^{-1}(u), x \mapsto \widehat{w}(x) = T_u L_x(w)$. More generally, let $w : U \to A(\Gamma)$ be a smooth section of the vector bundle $\pi : A(\Gamma) \to \Gamma_0$, defined on an open subset U of Γ_0. By using the above-described construction for every point $u \in U$, we can extend the section w into a smooth vector field $\widehat{w}$, defined on the open subset $\beta^{-1}(U)$ of Γ, by setting, for all $u \in U$ and $x \in \beta^{-1}(u)$:

$$\widehat{w}(x) = T_u L_x(w(u))$$

We have defined an injective map $w \mapsto \widehat{w}$ from the space of smooth local sections of $\pi : A(\Gamma) \to \Gamma_0$, into a subspace of the space of smooth vector fields defined on open subsets of Γ. The image of that map is the space of smooth vector fields $\widehat{w}$, defined on open subsets $\widehat{U}$ of Γ of the form $\widehat{U} = \beta^{-1}(U)$, where

U is an open subset of Γ_0, which satisfy the two properties:

1. $T\alpha \circ \widehat{w} = 0$,
2. for every x and $y \in \widehat{U}$ such that $\beta(x) = \alpha(y)$, $T_y L_x(\widehat{w}(y)) = \widehat{w}(xy)$.

These vector fields are called "left-invariant vector fields" on Γ.

The space of left-invariant vector fields on Γ is closed under the bracket operation. We can therefore define a composition law $(w_1, w_2) \mapsto \{w_1, w_2\}$ on the space of smooth sections of the bundle $\pi : A(\Gamma) \to \Gamma_0$ by defining $\{w_1, w_2\}$ as the unique section such that

$$\widehat{\{w_1, w_2\}} = [\widehat{w}_1, \widehat{w}_2]$$

Finally, we define the anchor map ρ as the map $T\beta$ restricted to $A(\Gamma)$. With that composition law and that anchor map, the vector bundle $\pi : A(\Gamma) \to \Gamma_0$ is a Lie algebroid, called the Lie algebroid of the Lie groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$.

We could exchange the roles of α and β and use right-invariant vector fields instead of left-invariant vector fields. The Lie algebroid obtained remains the same, up to an isomorphism.

When the Lie groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}}$ is a Lie group, its Lie algebroid is simply its Lie algebra.

The Lie Algebroid of a Symplectic Groupoid

Let $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ be a symplectic groupoid, with symplectic form ω. As we have seen above, its Lie algebroid $\pi : A \to \Gamma_0$ is the vector bundle whose fiber, over each point $u \in \Gamma_0$, is $\ker T_u\alpha$. We define a linear map $\omega_u^\flat : \ker T_u\alpha \to T_u^*\Gamma_0$ by setting, for each $w \in \ker T_u\alpha$ and $v \in T_u\Gamma_0$,

$$\left\langle \omega_u^\flat(w), v \right\rangle = \omega_u(v, w)$$

Since $T_u\Gamma_0$ is Lagrangian and $\ker T_u\alpha$ complementary to $T_u\Gamma_0$ in the symplectic vector space $(T_u\Gamma, \omega(u))$, the map $\omega_u^\flat$ is an isomorphism from $\ker T_u\alpha$ onto $T_u^*\Gamma_0$. By using that isomorphism for each $u \in \Gamma_0$, we obtain a vector bundle isomorphism of the Lie algebroid $\pi : A \to \Gamma_0$ onto the cotangent bundle $\pi_{\Gamma_0} : T^*\Gamma_0 \to \Gamma_0$.

As seen in Corollary 5, the submanifold of units Γ_0 has a unique Poisson structure Π for which $\alpha : \Gamma \to \Gamma_0$ is a Poisson map. Therefore, the cotangent bundle $\pi_{\Gamma_0} : T^*\Gamma_0 \to \Gamma_0$ to the Poisson manifold (Γ_0, Π) has a Lie algebroid structure, with the bracket of 1-forms as composition law. That structure is the same as the structure obtained as a direct image of the Lie algebroid structure of $\pi : A(\Gamma) \to \Gamma_0$, by the above-defined vector bundle isomorphism of $\pi : A \to \Gamma_0$ onto the cotangent bundle $\pi_{\Gamma_0} : T^*\Gamma_0 \to \Gamma_0$. The Lie algebroid of the symplectic groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ can therefore be identified with the Lie algebroid $\pi_{\Gamma_0} : T^*\Gamma_0 \to \Gamma_0$, with its Lie algebroid structure of cotangent bundle to the Poisson manifold (Γ_0, Π).

The Lie Algebroid of a Poisson Groupoid

The Lie algebroid $\pi : A(\Gamma) \to \Gamma_0$ of a Poisson groupoid has an additional structure: its dual bundle $\varpi : A(\Gamma)^* \to \Gamma_0$ also has a Lie algebroid structure, compatible in a certain sense (indicated below) with that of $\pi : A(\Gamma) \to \Gamma_0$.

The compatibility condition between the two Lie algebroid structures on the two vector bundles in duality $\pi : A \to M$ and $\varpi : A^* \to M$ can be written as follows:

$$d_*[X, Y] = \mathcal{L}(X)d_*Y - \mathcal{L}(Y)d_*X \qquad [21]$$

where X and Y are two sections of π, or, using the generalized Schouten bracket of sections of exterior powers of the Lie algebroid $\pi : A \to M$,

$$d_*[X, Y] = [d_*X, Y] + [X, d_*Y] \qquad [22]$$

In these formulas d_* is the generalized exterior derivative, which acts on the space of sections of exterior powers of the bundle $\pi : A \to M$, considered as the dual bundle of the Lie algebroid $\varpi : A^* \to M$.

These conditions are equivalent to the similar conditions obtained by exchange of the roles of A and A^*.

When the Poisson groupoid $\Gamma \overset{\alpha}{\underset{\beta}{\rightrightarrows}} \Gamma_0$ is a symplectic groupoid, we have seen that its Lie algebroid is the cotangent bundle $\pi_{\Gamma_0} : T^*\Gamma_0 \to \Gamma_0$ to the Poisson manifold Γ_0 (equipped with the Poisson structure for which α is a Poisson map). The dual bundle is the tangent bundle $\tau_{\Gamma_0} : T\Gamma_0 \to \Gamma_0$, with its natural Lie algebroid structure defined earlier.

When the Poisson groupoid is a Poisson Lie group (G, Π), its Lie algebroid is its Lie algebra $\mathcal{G}$. Its dual space $\mathcal{G}$ has a Lie algebra structure, compatible with that of $\mathcal{G}$ in the above-defined sense, and the pair $(\mathcal{G}, \mathcal{G}^*)$ is called a Lie bialgebra.

Conversely, if the Lie algebroid of a Lie groupoid is a Lie bialgebroid (i.e., if there exists on the dual vector bundle of that Lie algebroid a compatible structure of Lie algebroid, in the above-defined sense), that Lie groupoid has a Poisson structure for which it is a Poisson groupoid.

Integration of Lie Algebroids

According to Lie's third theorem, for any given finite-dimensional Lie algebra, there exists a Lie group whose Lie algebra is isomorphic to that Lie algebra. The same property is not true for Lie algebroids and Lie groupoids. The problem of

finding necessary and sufficient conditions under which a given Lie algebroid is isomorphic to the Lie algebroid of a Lie groupoid remained open for more than 30 years, although partial results were obtained. A complete solution of that problem was recently obtained by M Crainic and R L Fernandes. Let us briefly sketch their results.

Let $\pi : A \to M$ be a Lie algebroid and $\rho : A \to TM$ its anchor map. A smooth path $a : I = [0, 1] \to A$ is said to be admissible if, for all $t \in I$, $\rho \circ a(t) = (\mathrm{d}/\mathrm{d}t)(\pi \circ a)(t)$. When the Lie algebroid A is the Lie algebroid of a Lie groupoid Γ, it can be shown that each admissible path in A is, in a natural way, associated to a smooth path in Γ starting from a unit and contained in an α-fiber. When we do not know whether A is the Lie algebroid of a Lie groupoid or not, the space of admissible paths in A still can be used to define a topological groupoid $\mathcal{G}(A)$ with connected and simply connected α-fibers, called the Weinstein groupoid of A. When $\mathcal{G}(A)$ is a Lie groupoid, its Lie algebroid is isomorphic to A, and when A is the Lie algebroid of a Lie groupoid Γ, $\mathcal{G}(A)$ is a Lie groupoid and is the unique (up to an isomorphism) Lie groupoid with connected and simply connected α-fibers with A as Lie algebroid; moreover, $\mathcal{G}(A)$ is a covering groupoid of an open sub-groupoid of Γ. Crainic and Fernandes have obtained computable necessary and sufficient conditions under which the topological groupoid $\mathcal{G}(A)$ is a Lie groupoid, that is, necessary and sufficient conditions under which A is the Lie algebroid of a Lie groupoid.

See also: Classical *r*-Matrices, Lie Bialgebras, and Poisson Lie Groups; Lie Superalgebras and Their Representations; Lie Groups: General Theory; Nonequilibrium Statistical Mechanics (Stationary): Overview; Poisson Reduction.

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Liquid Crystals

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Liquid crystals represent an important state of matter, intermediate between regular solids with long-range positional order of atoms or molecules (often accompanied by the orientational order, as in the case of molecular crystals) and isotropic fluids with neither positional nor orientational long-range order. The basic feature of liquid crystals is orientational order of building units, which might be individual molecules or their aggregates, and complete or partial absence of the long-range positional order. Molecular interactions responsible for orientation order in liquid crystals are relatively weak (most liquid crystals melt into the isotropic phase at around 100–150 °C). As a result, the structural organization of liquid crystals, most importantly, the direction of molecular orientation, is very sensitive to the external factors, such as electromagnetic field and boundary conditions. This sensitivity opened the doors for applications of liquid crystals, including in information displays and flat-panel TVs.

Liquid crystals, discovered more than 100 years ago, represent nowadays one of the best studied classes of soft matter, along with colloids, polymer solutions and melts, gels and foams. There is an extensive literature on physical phenomena in liquid crystals, their chemical structure and material parameters, display applications, etc.

Thermotropic and Lyotropic Systems

Depending on the way the liquid crystalline state (also known as "mesophase") is produced, one distinguishes thermotropic and lyotropic liquid crystals. Thermotropic liquid crystalline state can exist in a certain temperature range for the materials made of strongly anisometric molecules, either elongated (calamitic molecules) or disk-like (discotic molecules). Upon heating, many substances of this type yield the following phase sequence: solid crystal–liquid crystal–isotropic fluid.

Lyotropic liquid crystals form only in the presence of a solvent, such as water or oil. Most commonly, lyotropic mesophases are formed by solutions of anisometric amphiphilic molecules (such as soaps, phospholipids, and surfactants). Amphiphilic molecules have two distinct parts: a (polar) hydrophilic head and a (nonpolar) hydrophobic tail (generally, an aliphatic chain). This feature gives rise to a special "self-organization" of amphiphilic molecules in solvents. Mesomorphic states also might be formed in the solutions of certain polymers; polymers might also form thermotropic (solvent-free) liquid crystals.

There are four basic types of liquid crystalline phases, classified according to the dimensionality of the translational correlations of building units: nematic (no translational correlations), smectic (1D correlations), columnar (2D correlations), and various 3D-correlated structures, such as cubic phases and blue phases.

"Uniaxial nematic," noted UN, is an optically uniaxial fluid phase. The unit vector along the optic axis is called the director $\boldsymbol{n}$, $\boldsymbol{n}^2 = 1$; it indicates the average orientation of the molecular axes (see **Figure 1**). Even when the molecules are polar, head-to-head overlapping and flip-flops establish centrosymmetric arrangement in the nematic bulk. Thus, $\boldsymbol{n}$ and $-\boldsymbol{n}$ are equivalent notations. It is important to realize that $\boldsymbol{n}$ specifies only the direction of orientation but not the degree of orientational order. In biaxial nematics (BN), the symmetry point group is one of a prism. A BN phase is characterized by three directors, $\boldsymbol{n}$, $\boldsymbol{l}$, and $\boldsymbol{m} = \boldsymbol{n} \times \boldsymbol{l}$, such that $\boldsymbol{n} \equiv -\boldsymbol{n}, \boldsymbol{l} \equiv -\boldsymbol{l}$, and $\boldsymbol{m} \equiv -\boldsymbol{m}$.

When the building unit (molecule or aggregate) is chiral, that is, not equal to its mirror image, UN might show a helicoidal structure. It is then called a cholesteric phase denoted Ch or N*. Note that UN, BN, and N* phases are liquid phases (no long-range correlations in molecular positions).

"Smectics" are layered phases with a quasi-long-range 1D translational order of centers of molecules in a direction normal to the layers (see **Figure 2**). This positional order is not exactly the long-range order as in regular 3D crystals: as shown by Landau and Peierls, the fluctuative displacements of layers in 1D lattice diverge logarithmically with the size of the sample. However, for regular materials with smectic period of the order of 1 nm, the effect is noticeable only on scales of 1 mm and larger. In smectic A (SmA), the molecules within the layers show fluid-like arrangement, with no long-range in-plane positional order; it is a uniaxial medium with the optic axis $\boldsymbol{n}$ perpendicular to the layers (see **Figure 2**). Some materials, such as octylcyanobiphenyl (see **Figure 1b**), show both UN and SmA phase (at somewhat lower temperatures). In the lyotropic version of SmA, the so-called lamellar L_α phase, the amphiphilic molecules arrange into bilayers. If the solvent is water, the exterior surfaces of the bilayer are formed by polar heads; the hydrophobic tails are

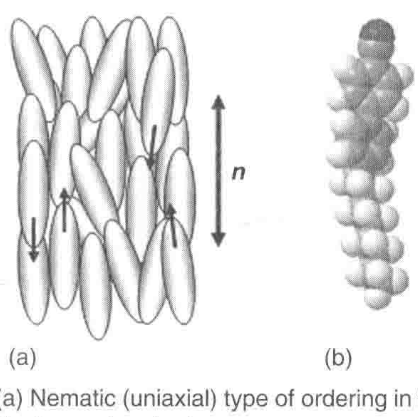


Figure 1 (a) Nematic (uniaxial) type of ordering in thermotropic liquid crystals; the molecular long axes are on average aligned along the director $\boldsymbol{n}$; (b) a molecule of octylcyanobiphenyl, a typical thermotropic liquid crystalline material capable of both nematic and SmA types of ordering.

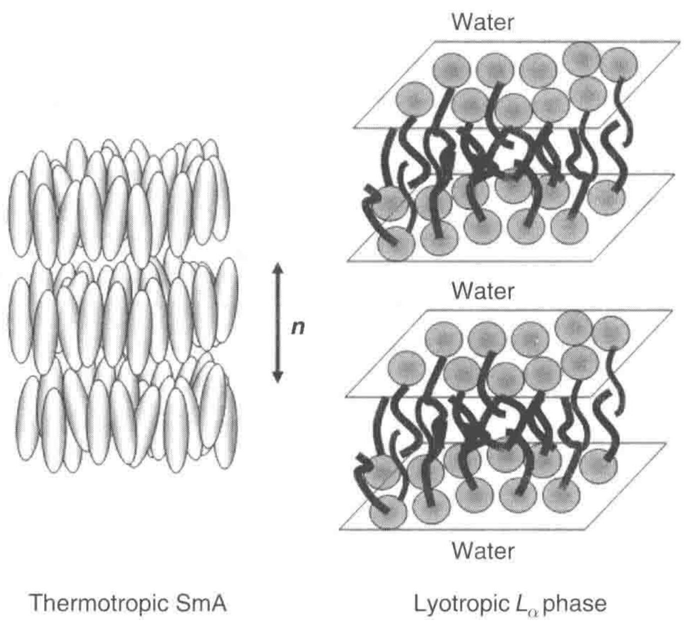


Figure 2 SmA type of ordering in the thermotropic SmA liquid crystal (left) and the lyotropic analog, L_α phase (right) formed by equidistant arrangement of amphiphilic bilayers in water.

hidden in the middle of the bilayer (note that membranes of many biological cells are organized in the similar way). The periodic structure of alternating surfactant and water layers gives rise to the L_α phase (see **Figure 2**). Interestingly, the structure might retain its smectic ordering even when strongly diluted, being stabilized by thermal fluctuations of bilayers.

Other types of smectics show in-plane order, caused, for example, by a collective tilt of the rod-like molecules with respect to the normals to the layers (the so-called SmC). In chiral materials, the tilt of the molecules might lead to the helicoidal structure; we do not consider them here, although the chiral SmC phase is of considerable interest for applications in fast-switching optical devices.

"Columnar phases" are most frequently formed by hexagonal packing of cylindrical aggregates, as in the case of thermotropic materials formed by disc-like molecules. The positional order is 2D only, as the intermolecular distances along the axes of the aggregates are not regular.

"3D-correlated structures" demonstrate a periodic structure along all three coordinates, but they are still different from the 3D crystals, as the periodicity is caused by the repetition of molecular orientations rather than by regular repetition of the molecular centers of mass. For example, in cubic lyotropic phases, the 3D network is formed by periodically curved layers of amphiphilic molecules; the molecules are free to move within the layers.

Order Parameter

The concept of an order parameter (OP) has emerged in its modern form in the Landau model of phase transitions and has been later expanded to describe other features such as topologically stable defects in the ordered media. The OP of the liquid crystal can be related to the anisotropy of macroscopic properties such as diamagnetic or dielectric susceptibility. Measuring these anisotropies allows one to determine the degree of orientational order. The magnetic measurements are especially convenient compared with their electric counterparts, as in this case the local field acting on the molecules differs very little from the external field. In UN, the components of the (symmetric) magnetic susceptibility tensor $\bar{\bar{\chi}}$ read in the frame in which the z-axis is parallel to the director $\boldsymbol{n}$, as

$$\bar{\bar{\chi}} = \begin{pmatrix} \chi_\perp & 0 & 0 \\ 0 & \chi_\perp & 0 \\ 0 & 0 & \chi_\parallel \end{pmatrix} \qquad [1]$$

The quantity $\chi_a = \chi_\parallel - \chi_\perp$ is called the anisotropy of the magnetic susceptibility. In most thermotropic UNs, $\chi_\parallel < 0$ and $\chi_\perp < 0$ (diamagnetism), and $\chi_a > 0$, so that $\boldsymbol{n}$ orients along the applied magnetic field. In the isotropic phase, $\chi_a = 0$; in UN, χ_a is determined by (1) molecular susceptibilities of individual molecules and (2) degree of molecular order. For the latter, one can chose the temperature-dependent quantity $s(T) = (1/2)\langle 3\cos^2\theta - 1\rangle$, where θ is the angle between the axis of an individual molecule and the director $\boldsymbol{n}$ and $\langle \ldots \rangle$ means an average over molecular orientations. The OP is thus the traceless symmetric tensor $\bar{\bar{Q}}$ with the components that vanish in the isotropic phase, and are proportional to χ_a in the UN phase:

$$\bar{\bar{Q}} = Q \begin{pmatrix} -\chi_a/3 & 0 & 0 \\ 0 & -\chi_a/3 & 0 \\ 0 & 0 & 2\chi_a/3 \end{pmatrix} \qquad [2]$$

One can choose the constant Q in such a way that in an arbitrary coordinate system, where $\chi_{ij} = \chi_\perp \delta_{ij} + \chi_a n_i n_j$,

$$Q_{ij} = s(T)\left(n_i n_j - \tfrac{1}{3}\delta_{ij}\right) \qquad [3]$$

The tensor OP allows one to describe the biaxial nematic phase as well:

$$Q_{ij} = s(T)\left(n_i n_j - \tfrac{1}{3}\delta_{ij}\right) + b(T)\left(l_i l_j - m_i m_j\right) \qquad [4]$$

where $\boldsymbol{n}$, $\boldsymbol{l}$, and $\boldsymbol{m}$ are three orthogonal directors and b is the "biaxiality parameter"; $b = 0$ in UN.

Elasticity of the Nematic Phase

In real samples of liquid crystals, the average molecular orientation changes from point to point because of the external fields, boundary conditions, presence of foreign particles, etc. The OP becomes spatially nonuniform, $Q_{ij}(\boldsymbol{r})$. In most problems of practical interest, the typical scale of distortions is much larger than the molecular scale; the deformations are weak in the sense that the scalar part of the OP, $s(T)$, remains constant despite the spatial gradients of the director field $\boldsymbol{n}(\boldsymbol{r})$.

The free-energy density associated with the (small) deformations of the UN, classified as splay, twist, and bend of the director (see **Figure 3**) writes in terms of the director gradients $n_{i,j} = (\partial n_i/\partial x_j)$ as

$$f_{\mathrm{FO}} = \tfrac{1}{2}K_1(\operatorname{div}\boldsymbol{n})^2 + \tfrac{1}{2}K_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n})^2 + \tfrac{1}{2}K_3(\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n})^2 \qquad [5]$$

and is known as the Frank–Oseen energy density with Frank elastic constants of splay (K_1), twist (K_2), and bend (K_3); all three are necessarily positive definite; the

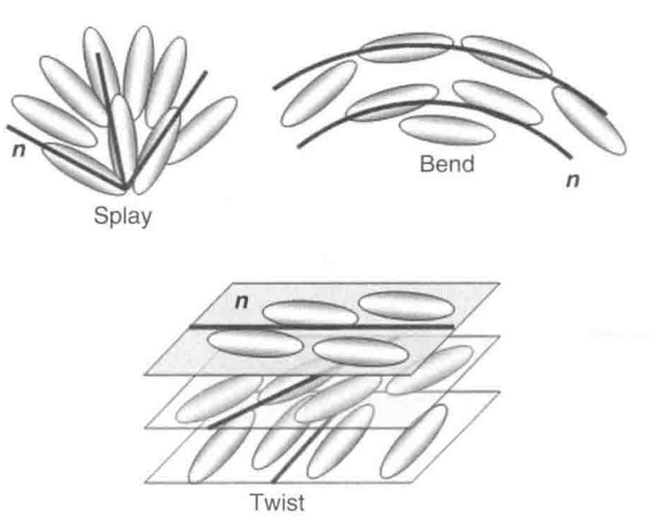


Figure 3 Basic types of director distortions in the bulk of the uniaxial nematic.

dimensionality is that of a force. The elastic constants can be estimated as the typical energy of molecular interactions responsible for the orientational order divided by the characteristic length (a molecular size): $K \sim U/l \sim k_B T/l \sim 4 \times 10^{-21}\text{J}/10^{-9} \sim 4\,\text{pN}$, which yields a good estimate for many thermotropic UNs, as the experimental values are between 1 and 10 pN. The energy density [5] is often supplemented with the so-called divergence terms:

$$f_{13} + f_{24} = K_{13}\,\text{div}(\boldsymbol{n}\,\text{div}\,\boldsymbol{n}) - K_{24}\,\text{div}(\boldsymbol{n}\,\text{div}\,\boldsymbol{n} + \boldsymbol{n} \times \text{curl}\,\boldsymbol{n}) \quad [6]$$

The K_{24} term can be re-expressed as a quadratic form of the first derivatives whereas the K_{13} term is proportional to the second derivatives $n_{i,jk}$ and thus might in principle be comparable to $f_{FO} \sim n_{i,j}n_{k,l}$. The volume integrals of these terms can be re-expressed as the surface integrals by virtue of the Gauss theorem (but only when the elastic moduli K_{13} and K_{24} are constant which might not be the case at certain interfaces and at the core of defects). Therefore, when one seeks for equilibrium director configurations by minimizing the total free-energy functional $\int(f_{FO} + f_{13} + f_{24})\text{d}V$, the K_{13} and K_{24} terms do not enter the Euler–Lagrange variational derivative for the bulk. However, they can contribute to the energy and influence the equilibrium director through boundary conditions at the surface. Usually, K_{24} term is retained when the system experiences a topological change of the director field. The K_{13} term is often neglected; very little is known about K_{13} value.

In the presence of external field, the free-energy density acquires additional terms. For example, for the magnetic field $\boldsymbol{B}$, the energy density [5], [6] should be supplemented by the term $-(1/2)\mu_0^{-1}\chi_a(\boldsymbol{B} \cdot \boldsymbol{n})^2$, where $\mu_0 = 4\pi \times 10^{-7}\,\text{Hm}^{-1}$ is the magnetic permeability of free space (magnetic constant).

The possibility to orient the director by an applied electric or magnetic field leads to numerous practical applications. Any actual liquid crystal cell is confined; say, by a pair of parallel glass plates. The molecular interactions between the liquid crystal and the boundary substrates are anisotropic. This anisotropy establishes one (sometimes more) preferred orientation of $\boldsymbol{n}$ at the boundary, the so-called "easy axis." The phenomenon is called the "surface anchoring." Orienting action of the substrates usually keeps the director uniform if the external field is absent. However, the external field can overcome both the "anchoring" at the surfaces and the elasticity of the nematic bulk and reorient the director. This is the "Frederiks effect," first discovered for the magnetic case. When the field is removed, the surface anchoring restores the original director structure. Thus, one can use the external field and surface anchoring to switch the liquid crystal orientation back and forth. The dielectric version of the effect is used in electrooptic devices, including displays. The liquid crystal is usually sandwiched between two transparent electroconductive plates (e.g., glass covered with indium tin oxide) coated with a suitable alignment layer. The voltage across the cell controls the director configuration and thus the optical properties of the cell.

Elasticity of the Smectic A Phase

For the SmA phase, the elastic free-energy density should be modified to take into account (1) restrictions that the layered structure imposes onto the director twist and bend, and (2) elastic cost of changes in the thickness of the layers:

$$f = \tfrac{1}{2}K_1(\text{div}\,\boldsymbol{n})^2 + \tfrac{1}{2}B\gamma^2 \quad [7]$$

where B is the Young modulus (layers compressibility modulus) and $\gamma = (d - d_0)/d_0$, the relative difference between the equilibrium period d_0 and the actual layer thickness measured along the director $\boldsymbol{n}$. The ratio of K_1 to B defines an important length scale

$$\lambda = \sqrt{K_1/B} \quad [8]$$

called "the penetration length"; λ is of the order of the layer separation but diverges when the system approaches the SmA–nematic transition. The splay constant K_1 in the SmA phase is of the same order as in a nematic phase stable at higher temperatures. With $\lambda \approx d_0 \approx (1 \div 3)\,\text{nm}$, one finds

$B \sim 10^6 \div 10^7\,\mathrm{N/m^2}$, a value that is 10^3 to 10^4 times smaller than the compressibility modulus in a solid.

The SmA elastic free-energy density is often written in terms of the mean curvature $H = (1/2)(\sigma_1 + \sigma_2)$ and the Gaussian curvature $G = \sigma_1\sigma_2$ of the layers:

$$f = \tfrac{1}{2}K_1(\sigma_1 + \sigma_2)^2 + \overline{K}\sigma_1\sigma_2 + \tfrac{1}{2}B\gamma^2 \qquad [9]$$

As compared with eqn [7], it is supplemented by the divergence saddle-splay term $\overline{K}$; $-2K_1 < \overline{K} \leq 0$ (for the system of flat layers to be energetically stable); $\sigma_1 = 1/R_1$ and $\sigma_2 = 1/R_2$ are the local values of the principal curvatures of the smectic layers.

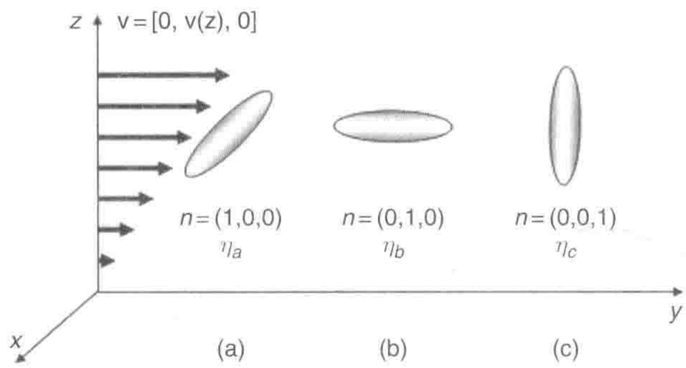


Figure 4 Miezowicz geometries for effective viscosities of the uniaxial nematic.

Dynamics

Liquid crystals are fluids; they can flow preserving the orientational order. Flow imposes an orientational torque on the liquid crystals. Most often, the director tends to realign along the direction of flow. There is also an inverse effect: director distortions can cause the flow. This "backflow" effect is of importance in liquid crystal displays. In the approximation of a constant scalar OP, the hydrodynamics of liquid crystals is described in terms of seven unknown variables: (1) mass density $\rho(\boldsymbol{r}, t)$, (2) three components of the velocity field $\boldsymbol{v}(\boldsymbol{r}, t)$, (3) energy density, and (4) two components of the director field $\boldsymbol{n}(\boldsymbol{r}, t)$. These variables are found from seven equations

1. conservation of mass,
2. three equations for the conserved components of the linear momentum,
3. entropy balance equation, and
4. two director dynamics equations.

In contrast to an isotropic fluid, the stress tensor depends not only on the gradients of the velocity, but also on the director components. UN phase should be characterized by five different viscosity constants. The number of viscosities reduces to three, when the director distortions are small. These three can be chosen as the effective viscosities for three idealized geometries of flow, also known as Miezowicz geometries, in which one assumes that the director is fixed (e.g., by a strong magnetic field) (see **Figure 4**):

When $\boldsymbol{n} = (1, 0, 0)$ is perpendicular to both the flow direction and the velocity gradient, the UN behaves as an isotropic fluid with a viscosity η_a; however, director fluctuations coupled with the certain values of the viscosity coefficients might destabilize the initial director orientation (see **Figure 4a**). When $\boldsymbol{n}$ is parallel to the flow (**Figure 4b**) or parallel to the velocity gradient (**Figure 4c**), the corresponding viscosities η_b and η_c are generally different from η_a and from each other; $\eta_b < \eta_a < \eta_c$ for a typical thermotropic UN material composed of the rod-like elongated molecules. The result $\eta_b < \eta_c$ can be explained by assuming that the friction correlates with the cross section of the molecules seen by the flow.

Topological Defects

Experimental Observations

When a thick UN sample (say, 100 μm thick) with no special aligning layers is viewed under the microscope, one usually observes a number of mobile flexible lines, the so-called disclinations. The disclinations are seen as thin and thick threads (see **Figure 5**). Thin threads strongly scatter light and show up as sharp lines. These are truly topologically stable defect lines, along which the nematic symmetry of rotation is broken. The disclinations are topologically stable in the sense that no continuous deformation can transform them into a uniform state, $\boldsymbol{n}(\boldsymbol{r}) = \text{const}$. Thin disclinations are singular in the sense that the director is not defined along the core of the defect line. Thick threads are line defects only in appearance; they are not singular disclinations. The director is smoothly curved and well defined everywhere, except, perhaps, at a number of point defects, the so-called hedgehogs (see **Figure 5**).

In thin UN samples (1–50 μm) with the director tangential to the bounding plates, the disclinations are often perpendicular to the plates. Under a microscope with two crossed polarizers, one can see the ends of the disclinations as centers with emanating pairs of dark brushes (see **Figure 6**) giving rise to the so-called "Schlieren texture." The dark brushes display the areas where $\boldsymbol{n}$ is either in

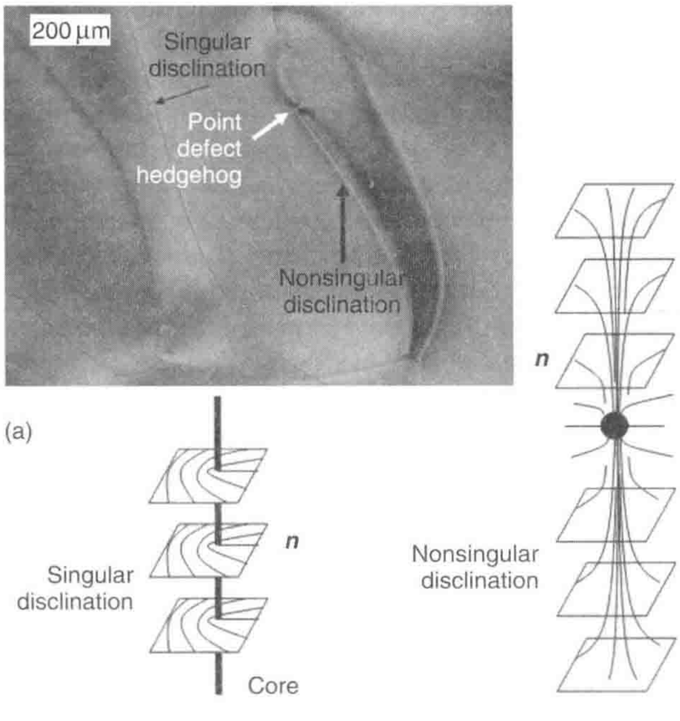


Figure 5 (a) Thin singular disclinations and thick nonsingular threads in the nematic (n-pentylcyanobiphenyle (5CB)) bulk. Crossed polarizers; (b, c) typical director configurations associated with thin and thick lines; thick lines are often associated with point defects in the nematic bulk – hedgehogs.

the plane of polarization of light or in the perpendicular plane. The director rotates by an angle $\pm\pi$ when one goes around the end of the disclination at the surface. Centers with four emanating brushes are also observed; they correspond to point defects located at the surface, the so-called boojums, (see **Figure 6**). The director undergoes a $\pm 2\pi$ rotation around these four-brush centers. The principal difference between the centers with two brushes (ends of singular lines) and centers with four brushes (surface point defects) can be seen after a gentle shift of one of the bounding plates with respect to the other. Upon shear-induced separation in the plane of observation, the centers with two brushes are clearly seen as connected by a singular trace – disclination, while the centers with four brushes separate without a visible singularity between them.

The intensity of linearly polarized light coming through a uniform UN slab depends on the angle β between the polarization direction and the projection of the director $\boldsymbol{n}$ onto the slab's plane:

$$I = I_0 \sin^2 2\beta \sin^2 \left[\frac{\pi h}{\lambda}\left(n_{\mathrm{e,eff}} - n_{\mathrm{o}}\right)\right] \quad [10]$$

where I_0 is the intensity of incident light, λ is the wavelength of the light, $n_{\mathrm{e,eff}}$ is the effective refractive index that depends on the ordinary index n_{o}, extraordinary index n_{e}, and the director orientation. Equation [10] allows one to relate the number $|k|$ of director rotations by $\pm 2\pi$ around the defect core, to the number B of brushes:

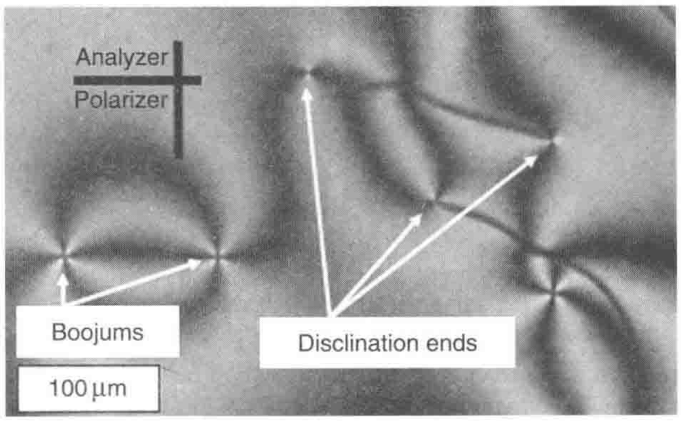


Figure 6 Schlieren texture of a thin (13 μm) slab of 5CB. Centers with two and four brushes are the ends of singular disclinations and point defects – boojums, respectively. Tangential director orientation. Crossed polarizers.

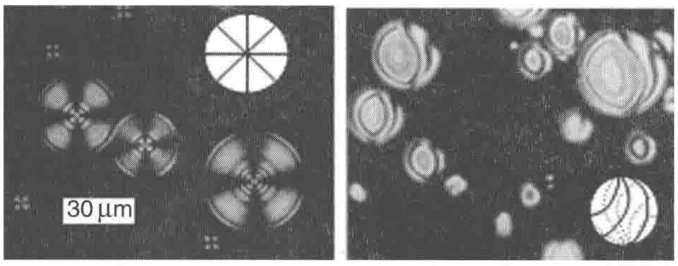
$$|k| = B/4 \quad [11]$$

Taken with a sign that specifies the direction of rotation, k is called the "strength of disclination," and is related to a more general concept of a topological charge (but does not coincide with it). Note that $I = 0$ when $\boldsymbol{n}$ is perpendicular to the plates (so-called homeotropic state), as $n_{\mathrm{e,eff}} = n_{\mathrm{o}}$. The homeotropic state is used as one of the ground states in modern flat-panel TV sets. By applying the electric field, one tilts the director so that $n_{\mathrm{e,eff}} \neq n_{\mathrm{o}}$ and the cell (or the corresponding pixel in the liquid crystal panel) becomes transparent.

Nematic Droplets

When left intact, textures with defects in flat samples relax into a more or less uniform state. Disclinations with positive and negative k find each other and annihilate. There are, however, situations when the equilibrium state requires topological defects. Nematic droplets suspended in an isotropic matrix such as glycerin, water, polymer, etc., (see **Figure 7**) and inverted systems, such as water droplets in a nematic matrix are the most evident examples.

Consider a spherical nematic droplet of a radius R and the balance of the surface anchoring energy $\sim W_a R^2$ (W_a is the surface anchoring coefficient), and the elastic energy $\sim KR$; K is some averaged Frank constant. Small droplets with $R << K/W_a$ avoid spatial variations of $\boldsymbol{n}$ at the expense of violated boundary conditions. In contrast, large droplets, $R >> K/W_a$, satisfy boundary conditions by aligning $\boldsymbol{n}$ along the



(a) (b)

Figure 7 Polarizing-microscope texture of spherical nematic droplets suspended in glycerin. (a) The director configuration is radial and normal to the spherical surface; the inset shows the point-defect hedgehog in the center of the droplet. (b) Tangential director orientation at the interface results in the bipolar structure with two defects-boojums at the poles. The director is twisted because of the smallness of the twist elastic constant as compared to the splay and bend constants.

preferred direction(s) at the surface. Since the surface is a sphere, the result is the distorted director in the bulk, for example, a radial hedgehog when the surface orientation is normal (see **Figure 7**). The characteristic radius R is macroscopic (microns), as $K \sim 10\,\mathrm{pN}$ and $W_a \sim 10^{-5}$–$10^{-6}\,\mathrm{J\,m^{-2}}$. Point defects in large nematic droplets must satisfy restrictions on their topological characteristics that have their roots in the Poincaré and Gauss theorems of differential geometry.

Topological Classification of Defects in UN

The language of topology, or, more precisely, of homotopy theory, allows one to associate the character of ordering of a medium and the types of defects arising in it, to find the laws of decay, merger and crossing of defects, to trace out their behavior during phase transitions, etc. The key point is occupied by the concept "of topological invariant," also called a "topological charge," which is inherent in every defect. The stability of the defect is guaranteed by the conservation of its charge. Homotopy classification of defects includes three steps.

First, one defines the OP of the system. In a nonuniform state, the OP is a function of coordinates.

Second, one determines the OP (or degeneracy) space $\boldsymbol{R}$, that is, the manifold of all possible values of the OP that do not alter the thermodynamical potentials of the system. In the UN, $\boldsymbol{R}$ is a unit sphere denoted S^2/Z_2 (also called the projective plane RP_2) with pairs of diametrically opposite points being identical. Every point of S^2/Z_2 represents a particular orientation of $\boldsymbol{n}$. Since $\boldsymbol{n} \equiv -\boldsymbol{n}$, any two diametrically opposite points at S^2/Z_2 describe the same state.

The function $\boldsymbol{n}(\boldsymbol{r})$ maps the points of the nematic volume into S^2/Z_2. The mappings of interest are those of i-dimensional "spheres" enclosing defects. A line defect is enclosed by a linear contour, $i=1$; a point defect is enclosed by a sphere, $i=2$, etc.

Third, one defines the homotopy groups $\pi_i(\boldsymbol{R})$. The elements of these groups are mappings of i-dimensional spheres enclosing the defect in real space into the OP space. To classify the defects of dimensionality t' in a t-dimensional medium, one has to know the homotopy group $\pi_i(\boldsymbol{R})$ with $i = t - t' - 1$.

Each element of $\pi_i(\boldsymbol{R})$ corresponds to a class of topologically stable defects; all these defects are equivalent to one another under continuous deformations. The elements of homotopy groups are topological charges of the defects. For UN, the homotopy group $\pi_1(S^2/Z_2) = Z_2 = \{0, 1/2\}$ is composed of two elements; there is thus only one class of topologically stable defects (that appear as thin singular lines under the microscope, see **Figure 5**) with the addition rules $1/2 + 1/2 = 0$ and $1/2 + 0 = 1/2$ describing interaction of disclinations. The topological point defects in the bulk (hedgehogs) are described by the second homotopy group, $\pi_2(S^2/Z_2) = Z = \{0, 1, 2, \ldots\}$, and can be labeled by integer topological charges. The simplest point defect is a "radial" hedgehog, seen in the center of the radial droplet (see **Figure 7a**). Boojums are special point defects that, in contrast to hedgehogs, can exist only at the boundary of the medium (see **Figure 7b**).

The relative stability of stable disclinations depends on the Frank elastic constants of splay (K_{11}), twist (K_{22}), bend (K_{33}) and saddle-splay (K_{24}) in the Frank–Oseen elastic free-energy density functional; the role of the elastic constant K_{13} in the structure of defects is not clarified yet.

Consider the simplest case of "planar" disclinations with $\boldsymbol{n}$ perpendicular to the line. In this case, the K_{24}-term in the line's energy is zero. Assuming $K_{11} = K_{22} = K_{33} = K$, by minimizing the bulk integral of [5], one finds the equilibrium director configuration around the line of strength k

$$\boldsymbol{n} = \{\cos[k\varphi + c], \sin[k\varphi + c], 0\} \qquad [12]$$

where $\varphi = \arctan(y/x)$, x and y are Cartesian coordinates normal to the line, c is a constant. The energy per unit length of a straight planar disclination is

$$F_{1l} = \pi K k^2 \ln\frac{L}{r_c} + F_c \qquad [13]$$

where L is the characteristic size of the system, r_c and F_c are, respectively, the radius and the energy of the disclination core, a region in which the distortions are too strong to be described by a phenomenological theory.

The restriction of planar director distortions does not allow the model to grasp the crucial difference between half-integer and integer k's. The lines of integer k, as already discussed, are fundamentally unstable, as the director can be reoriented along the axis. This "escape in the third dimension," is usually energetically favorable, since the singular core is eliminated. When opposite directions of the "escape" meet, a point defect hedgehog is formed, as illustrated in **Figure 5c**.

Unlike point defects such as vacancies in solids, topological point defects in nematics cause disturbances over the whole volume. The curvature energy of the point defect is proportional to the size R of the system. For example, for the radial hedgehog with $\mathbf{n}=(x,y,z)/\sqrt{x^2+y^2+z^2}$, and the hyperbolic hedgehog with $\mathbf{n}=(-x,-y,z)/\sqrt{x^2+y^2+z^2}$, one finds, respectively,

$$F_{\rm rh}=8\pi R(K_{11}-K_{24})+F_{\rm cr} \quad \text{and}$$

$$F_{\rm hh}=8\pi R\left(\frac{K_{11}}{5}+\frac{2K_{33}}{15}+\frac{K_{24}}{3}\right)+F_{\rm ch} \qquad [14]$$

Defects in Smectics

Layered structure of smectics leads to linear defects of positional order, dislocations, in addition to disclinations. There is also a special class of distortions known as focal conic domains (FCDs) that are associated with large-scale curvatures of layers. Imagine that because of the boundary conditions, flow, or the external fields, the smectic layers are curved over the scale much larger than the thickness of the layers. It is easy to see from eqn [9] that the curved layers will prefer to maintain their equidistance, as the curvature energy is much smaller than the layers dilation energy at the large scales of deformations. Generally, the family of equidistant curved surfaces is associated with the focal surfaces at which the principal curvatures diverge. These focal surfaces are thus energetically very costly. A radical way to reduce the elastic energy would be to decrease the dimensionality of the focal surfaces, say, by transforming them into lines and points. The latter case corresponds simply to a system of concentric spherical layers. The former is more complicated and corresponds to FCDs in which the focal surfaces are represented by pairs of confocal lines: ellipse and hyperbola (limiting case: circle and straight line), and the pair of confocal parabolae. Experiments confirm that the FCDs are the most frequent type of structural deformations in smectic materials see **Figure 8**.

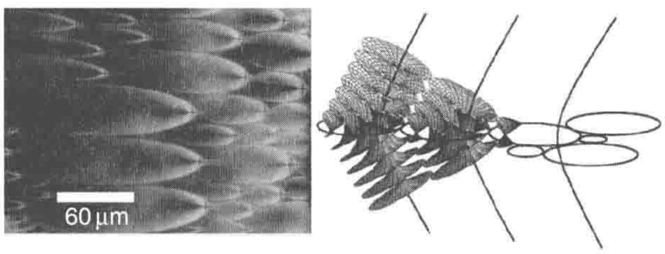


Figure 8 SmA phase with FCDs based on the confocal pairs of ellipses and hyperbolas; the scheme on the right shows the arrangement of the elliptic bases and smectic layers wrapped around the confocal pairs of defects. Reproduced from Lavrentovich OD (2003) In: Arodz *et al.* (eds.) *Patterns of Symmetry Breaking.* Dordrecht: Kluwer Academic Publishers, with kind permission of Springer Science and Business Media.

Conclusion

To summarize, over the last few decades, liquid crystals transformed from a mysterious and curious form of condensed matter into a key technological material, thanks to the progress in the understanding of their elastic, optical, and viscous properties. However, the intrinsic complexity of these materials still leaves plenty of room for further studies, not only of an applied nature, but also fundamental. In the field of thermotropic liquid crystals, researchers continue to discover new types of structural organization, such as the phases formed by "banana-shaped" molecules that are dramatically different from the phases formed by "regular" rod-like and disk-like molecules. There is a continuous work to sharpen our understanding of even the "old" problems, such as mechanisms of surface alignment, nature and quantitative values of the elastic constants K_{13}, K_{24}, and $\bar{K}$. Even in the case of the electric Frederiks effect that is at the heart of modern applications, the search continues as the corresponding process of director reorientation is generally very complex. In addition to the dielectric torque, it is controlled by various factors, for example, a nonlocal character of the electric field in the anisotropic medium, finite electric conductivity, flexoelectric effect (i.e., electric polarization brought about by the director deformations), surface electric polarization at the bounding plates, dependence of the dielectric and other material properties on the frequency of the applied field which might be comparable with the

characteristic frequency of dielectric relaxation, coupling of the director reorientation and the material's flows, appearance of topological defects, etc. Many research efforts nowadays are focused on composite systems, such as liquid crystal colloids and polymer–liquid crystal composites. Over the next decade or so, one would expect that the emphasis in fundamental studies will gradually shift from the thermotropic liquid crystals to their lyotropic counterparts, as the lyotropic type of orientational order is featured by many systems of biological significance, such as solutions of DNA, f-actin, etc.

See also: Non-Newtonian Fluids; Topological Defects and Their Homotopy Classification.

Further Reading

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Ljusternik–Schnirelman Theory

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Introduction

Using Lagrange multipliers, the smallest and the largest eigenvalue of a symmetric quadratic form

$$Q(u) = \sum_{j,k=1}^{n} a_{jk} u_j u_k \quad (a_{jk} = a_{kj})$$

can be obtained by minimizing and maximizing Q on the unit sphere $S^{n-1} = \{u \in \mathbb{R}^n : \|u\| = 1\}$. If the corresponding extremum is reached at u^*, then u^* is an associated eigenvector.

In the setting of integral or partial differential equations, a "recursive variational method" has been proposed to determine all the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and corresponding eigenvectors $u^1, u^2, \ldots, u^n$ of Q or, in modern terms, of the associated symmetric matrix $A = (a_{ij})$:

$$\lambda_1 = \min_{\|u\|=1} Q(u) \quad (= Q(u^1))$$

$$\lambda_j = \min_{\|u\|=1, u\cdot u^1=0, \ldots, u\cdot u^{j-1}=0} Q(u)$$
$$(= Q(u^j)) \quad (j = 2, \ldots, n)$$

Further considerations have led to a nonrecursive minimum–maximum principle:

$$\lambda_j = \min_{\{X^j \subset \mathbb{R}^n : \dim X^j = j\}} \max_{\{u \in X^j : \|u\|=1\}} Q(u) \quad (1 \leq j \leq n)$$

and to a dual maximum–minimum principle (Weyl):

$$\lambda_j = \max_{\{p_1, \ldots, p_{j-1} \in \mathbb{R}^n\}} \min_{\{\|u\|=1, u\cdot p_i = 0, 1 \leq i \leq j-1\}} Q(u)$$
$$(1 \leq j \leq n)$$

These principles have been widely used in various existence and approximation questions of mathematical physics, and extensions have been made to the abstract setting of symmetric bilinear forms in Hilbert spaces.

Around 1930, Ljusternik and Schnirelman have extended this theory beyond the frame of quadratic forms, replacing Q by a differentiable real-valued function f and the unit sphere by a finite-dimensional compact differentiable manifold M. Their aim was the obtention of the "critical points" of f on M, that is, the points $u \in M$ where the differential $f'(u)$ of f at u (as a linear functional on the tangent space $T_u M$ to M) is equal to zero, and of the corresponding critical values, that is, the values of f at critical points. When M is a sphere, the

critical points are nontrivial solutions of the equation

$$f'(u) = \lambda u \qquad [1]$$

for some $\lambda \in \mathbb{R}$ (nonlinear eigenvalue problem). Ljusternik and Schnirelman have replaced the dimension of the vector spaces occurring in the minimum–maximum principle for eigenvalues by the concept of "category" of a closed set A in a topological space X. An early success of their approach was the existence of three geometrically distinct closed geodesics without self-intersections on any compact surface of genus zero. In 1960, their theory has been extended to infinite-dimensional manifolds and to other measures of the "size" of a set than the category, allowing many theoretical developments as well as various applications to nonlinear differential equations.

Ljusternik–Schnirelman Category

Let X be a topological space (e.g., a normed vector space, or a differentiable manifold, or a metric space), and A a closed subset of X. The category of A in X, $\mathrm{cat}_X(A)$, is the least integer k such that A can be written as $\bigcup_{j=1}^{k} A_j$, with A_j closed and contractible in X, that is, continuously deformable in X into a single point. If no such k exists, one sets $\mathrm{cat}_X(A) = +\infty$. We write $\mathrm{cat}(X)$ for $\mathrm{cat}_X(X)$. For example, if X is contractible (in itself), $\mathrm{cat}(X) = 1$. This is the case for any normed space X. For the hypersphere, $\mathrm{cat}_{\mathbb{R}^n}(S^{n-1}) = 1$, but $\mathrm{cat}(S^{n-1}) = 2$.

The Ljusternik–Schnirelman category satisfies the following properties, which are not too difficult to prove. If $A, B \subset X$ are closed,

1. $\mathrm{cat}_X(A) = 0$ if and only if $A = \emptyset$;
2. if $A \subset B, \mathrm{cat}_X(A) \le \mathrm{cat}_X(B)$;
3. $\mathrm{cat}_X(A \cup B) \le \mathrm{cat}_X(A) + \mathrm{cat}_X(B)$;
4. if $\eta: [0,1] \times X \to X$ is a continuous deformation of $X (\eta(0, A) = A), \mathrm{cat}_X(A) \le \mathrm{cat}_X(\eta(1, A))$; and
5. if X is a finite-dimensional manifold and $A \subset X$ is compact, there is a neighborhood B of A such that $\mathrm{cat}_X(B) = \mathrm{cat}_X(A)$.

Computing or even estimating the category of a given set is in general difficult, requiring techniques of algebraic topology. In particular, one can show that, for the n-torus $\mathbb{T}^n = S^1 \times S^1 \times \cdots \times S^1$ (n times), $\mathrm{cat}(\mathbb{T}^n) = n + 1$, and for the n-dimensional projective space $\mathbb{P}^n = S^n/\mathbb{Z}^2$, obtained by identifying the antipodal points of $S^n, \mathrm{cat}(\mathbb{P}^n) = n + 1$. It is clear that a set of category p must contain at least p points. If X is connected, any compact subset of category $p + 1$ has (topological) dimension larger or equal to p.

Ljusternik–Schnirelman Minimax Method

The Ljusternik–Schnirelman category of M provides a lower bound for the number of critical points of a smooth function f on suitable finite-dimensional manifolds M. Namely, if M is a compact Riemannian C^2-manifold without boundary, any $f \in C^2(M, \mathbb{R})$ has at least $\mathrm{cat}(M)$ distinct critical points, with critical values

$$c_k = \inf_{A \in \mathcal{A}_k} \sup_{u \in A} f(u) \quad (1 \le k \le \mathrm{cat}(M)) \qquad [2]$$

where

$$\mathcal{A}_k = \{A \subset M : A \text{ closed}, \mathrm{cat}_M(A) \ge k\} \\ (1 \le k \le \mathrm{cat}(M)) \qquad [3]$$

A fundamental technique in the proof is a deformation lemma along the trajectories of the gradient system associated to f (method of steepest descent). If ∇f denotes the gradient of f in the Riemannian structure of M, the Cauchy problem for the gradient system

$$\frac{\mathrm{d}\eta}{\mathrm{d}t} = -\nabla f(\eta), \quad \eta(0) = u \qquad [4]$$

has a unique globally defined continuous solution $\eta(t, u)$, which is such that

$$f(\eta(1, u)) - f(u) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} f(\eta(t, u))\, \mathrm{d}t \\ = -\int_0^1 \|\nabla f(\eta(t, u))\|^2\, \mathrm{d}t \qquad [5]$$

Notice that, by property (4) of the category, each deformation by η of a set in $\mathcal{A}_j$ remains in $\mathcal{A}_j$. For $c \in \mathbb{R}$, define

$$f^c := \{u \in M : f(u) \le c\} \\ K_c := \{u \in M : \nabla f(u) = 0, f(u) = c\} \qquad [6]$$

From [5] it follows that given $c \in \mathbb{R}$ and an open neighborhood U_c of K_c, one has $\eta(1, f^{c+\varepsilon} \setminus U_c) \subset f^{c-\varepsilon}$ for all sufficiently small $\varepsilon > 0$. This implies that if $c := c_j = c_{j+1} = \cdots = c_{j+q}$ for some $q \ge 0$, then $\mathrm{cat}_M(K_c) \ge q + 1$. Assume, by contradiction, that $\mathrm{cat}_M(K_c) \le q$, let U_c be an open neighborhood of K_c such that $\mathrm{cat}_M(U_c) = \mathrm{cat}_M(K_c)$ ($U_c = \emptyset$ if $q = 0$), $\varepsilon > 0$ such that $\eta(1, f^{c+\varepsilon} \setminus U_c) \subset f^{c-\varepsilon}$, and $A \in \mathcal{A}_{j+q}$ such that $\sup_A f \le c + \varepsilon$, that is, $A \subset f^{c+\varepsilon}$. Then

$$\mathrm{cat}_M(\eta(1, A \setminus U_c)) \ge \mathrm{cat}_M(A \setminus U_c) \\ \ge \mathrm{cat}_M(A) - \mathrm{cat}_M(U) \ge j$$

giving the contradiction $c \le \sup_{\eta(1,A)} f \le c - \varepsilon$.

Notice that, for each j, $c_j = \inf\{c \in \mathbb{R} : \mathrm{cat}_M(f^c) \ge j\}$, which shows that the c_j are precisely those levels of f where $\mathrm{cat}_M(f^c)$ changes. The presence of critical values is detected by changes in the topology of the

sublevel sets f^c when c varies, a common feature of many techniques for finding critical points of functions.

A direct consequence is that for each even $f \in C^2(\mathbb{R}^n, \mathbb{R})$, system [1] has at least n pairs of solutions $(u, -u)$ with $\|u\| = 1$. Indeed, the solutions of [1] are the critical points of f on S^{n-1}. As f takes the same values at antipodal points, it is well defined on the projective space $\mathbb{P}^{n-1}$, and $\operatorname{cat}(\mathbb{P}^{n-1}) = n$.

The Ljusternik–Schnirelman theorem can be extended to the C^1-situation. The category of M gives a lower bound for the number of critical points of f on the closed manifold M. If $\operatorname{Crit}(M)$ denotes the minimum of the number of critical points of all C^1-functions on M, so that $\operatorname{Crit}(M) \geq \operatorname{cat}(M)$, an interesting question is to estimate the gap $\operatorname{Crit}(M) - \operatorname{cat}(M)$. For M closed connected, $\operatorname{Crit}(M) \leq \dim(M) + 1$ (Takens). If $\operatorname{Crit}(M) = 2$, M is homeomorphic to a sphere, so that the equality $\operatorname{Crit}(S) = \operatorname{cat}(S)$ for homotopy spheres is equivalent to Poincaré's conjecture! Manifolds with $\operatorname{Crit}(M) = \operatorname{cat}(M) + 1$ are known, but not with $\operatorname{Crit}(M) > \operatorname{cat}(M) + 1$.

Ljusternik–Schnirelman Theory in Infinite-Dimensional Manifolds

The main difficulty in extending the results of the previous section to functions defined on infinite-dimensional manifolds lies in the lack of compactness. J T Schwartz and Palais have shown that such an extension is possible for functions f satisfying on M a compactness property (allowing an infinite-dimensional deformation lemma), now referred to as the Palais–Smale condition: each sequence (u_k) with $(f(u_k))$ bounded and $\lim_{k\to\infty} \nabla f(u_k) = 0$ has a convergent subsequence. Such a condition can be localized at level c by replacing the boundedness of $(f(u_k))$ by $\lim_{k\to\infty} f(u_k) = c$. The infinite-dimensional extension of Ljusternik–Schnirelman's theorem goes as follows: Let M be an infinite-dimensional Riemannian (or even Finsler) connected complete manifold of class C^1 without boundary. Any $f \in C^1(M, \mathbb{R})$ bounded from below and satisfying Palais–Smale condition has at least $\operatorname{cat}(M)$ distinct critical points.

A simple application can be given to the periodic solutions of period T (T-periodic solutions) of Lagrangian systems

$$u'' + \nabla V(u) = h(t) \qquad [7]$$

where $V \in C^1(\mathbb{R}^n, \mathbb{R})$, 2π-periodic in each component $u_j (1 \leq j \leq n)$, h is continuous, T-periodic and has mean value $\bar{h}$ equal to zero. By the least action principle, the T-periodic solutions of [7] are the critical points of the action functional

$$f(u) = \int_0^T \left[\frac{\|u'(t)\|^2}{2} - V(u(t)) + h(t)u(t)\right] \mathrm{d}t$$

on the Hilbert space H_T^1 obtained by completion of the space of T-periodic C^1 functions for the norm associated with the inner product

$$\langle u, v\rangle := \int_0^T u(t) \cdot v(t)\, \mathrm{d}t + \int_0^T u'(t) \cdot v'(t)\, \mathrm{d}t$$

It follows easily from condition $\bar{h} = 0$ that f is bounded from below and that $f(u + 2\pi e^j) = f(u)$ for all $u \in H_T^1$, with e^j the jth unit vector in $\mathbb{R}^n (1 \leq j \leq n)$. Consequently, we can see f as defined on the Riemannian manifold $\mathbb{T}^n \times \widetilde{H_T^1}$, where $\widetilde{H_T^1} = \{u \in H_T^1 : \bar{u} = 0\}$. It is easy to show that $\operatorname{cat}(\mathbb{T}^n \times \widetilde{H_T^1}) = \operatorname{cat}(\mathbb{T}^n) = n + 1$ and that f satisfies Palais–Smale condition on $\mathbb{T}^n \times \widetilde{H_T^1}$. Consequently, system [7] has at least $n + 1$ geometrically distinct T-periodic solutions. The same result holds for the more general systems

$$Mu'' + Au + \nabla F(u) = h(t)$$

occurring in the theory of multipoint Josephson junctions or in space discretizations of the sine-Gordon equation. In particular, the classical forced pendulum equation

$$u'' + a \sin u = h(t)$$

has at least two geometrically distinct T-periodic solutions when h is T-periodic and $\bar{h} = 0$, a result first proved, in a different way, by Mawhin and Willem.

Another way to study nonlinear eigenvalue problems of the form

$$f'(u) = \lambda g'(u)$$

in a Hilbert or a suitable reflexive Banach space X is based upon a Rayleigh–Ritz approximation through a sequence of finite-dimensional problems, where the classical theory is applied. Conditions upon $f, g \in C^1(X, \mathbb{R})$ are given, generalizing Ljusternik–Schnirelman's ones, which ensure the existence of infinitely many solutions. Again, some compactness is needed to justify the limit process, and expressed by some assumptions upon f and g too lengthy to be reproduced here. The following application is exemplary. Let $\Omega \subset \mathbb{R}^N$ be a bounded domain and $X = W_0^{1,p}(\Omega)$, $p > 1$, be the Sobolev space of functions $u : \Omega \to \mathbb{R}$ obtained as the completion of the smooth functions with compact support

in Ω for the norm $\|u\|_{1,p} = (\int_\Omega \|\nabla u\ (x)\|^p\,dx)^{1/p}$. Define the functionals f and g on $W_0^{1,p}(\Omega)$ by

$$f(u) = \int_\Omega \|\nabla u(x)\|^p dx, \quad g(u) = \int_\Omega |u(x)|^p dx$$

The critical points of f on $\{u \in X : g(u) = 1\}$ correspond to the nontrivial solutions of the Dirichlet eigenvalue problem

$$\Delta_p u = \lambda |u|^{p-2} u \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega \qquad [8]$$

for the p-Laplacian operator Δ_p defined by

$$\Delta_p u(x) := \nabla \cdot \left(\|\nabla u(x)\|^{p-2} \nabla u(x) \right)$$

which occurs in the modelization of various problems in a porous medium. An eigenvalue is any $\lambda \in \mathbb{R}$ such that problem [8] has a nontrivial solution. The Ljusternik–Schnirelman technique implies the existence of a sequence of eigenvalues going to infinity, with the usual minimax characterization. When $N = 1$, direct computations show that this sequence gives all eigenvalues, but the problem remains open for $N \geq 2$. The corresponding forced problem

$$\Delta_p u - \lambda |u|^{p-2} u = h(x) \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

is always solvable (although not uniquely) when λ is not an eigenvalue, but solvability conditions at the higher eigenvalues (Fredholm alternative) remain almost *terra incognita*.

Index Theories and Critical Points of Symmetric Functionals on a Banach Space

Closely related to the Ljusternik–Schnirelman category is the concept of index associated to the action of a compact topological group G on a normed space X, that is, to a continuous map $G \times X \to X, [g, u] \mapsto gu$ such that $1 \cdot u = u, (gh)u = g(hu)$, $u \mapsto gu$ is linear. The action is isometric if $\|gu\| = \|u\|$, $A \subset X$ is invariant if $gA = A$ for all $g \in G$, $f : X \to \mathbb{R}$ is invariant if $f \circ g = f$ for all $g \in G$, and $h : X \to X$ is equivariant if $g \circ h = h \circ g$ for each $g \in G$. Let $\mathrm{Fix}\, G = \{u \in X : gu = u \text{ for all } g \in G\}$. The aim of an index is to measure the size of invariant sets. Explicitly, an index theory associates to each closed invariant subset A of X a non-negative (possibly infinite) integer G-ind(A), its G-index, such that

1. G-ind$(A) = 0$ if and only if $A = \emptyset$;
2. if $R : A \to B$ is equivariant and continuous, G-ind$(A) \leq$ G-ind(B);
3. G-ind$(A \cup B) \leq$ G-ind(A) + G-ind(B); and
4. if A is compact, there is a closed invariant neighborhood U of A such that G-ind$(U) =$ G-ind(A).

A first example of index is Krasnosel'skii's genus or $\mathbb{Z}_2$-index which corresponds to the action $0 \cdot u = u, 1 \cdot u = -u$ of $G = \mathbb{Z}_2$. The invariant sets are the ones symmetric with respect to the origin and $\mathbb{Z}_2$-ind(A) is defined by $\mathbb{Z}_2$-ind$(\emptyset) = 0$ and, for $A \neq \emptyset$, as the smallest integer k such that there exists an odd $h \in C(A, \mathbb{R}^k \setminus \{0\})$. A consequence of the Borsuk–Ulam theorem in algebraic topology is that any symmetric bounded neighborhood of the origin in $\mathbb{R}^n$ has $\mathbb{Z}_2$-index equal to n. Furthermore, for a compact $A \subset \mathbb{R}^n \setminus \{0\}$ symmetric with respect to the origin, and $\widetilde{A} = A/\mathbb{Z}_2$ (A with antipodal points identified), one has $\mathbb{Z}_2$-ind$(A) = \mathrm{cat}_{\mathbb{R}^n \setminus \{0\}}(\widetilde{A})$.

A second example, the S^1-index, is important in the study of periodic solutions of autonomous Hamiltonian systems. S^1-ind$(\emptyset) = 0$ and for a nonempty closed invariant $A \subset X$, S^1-ind(A) is defined as the smallest integer k such that there exists a positive integer n and $h \in C(A, \mathbb{C}^k \setminus \{0\})$ with $h \circ g = g^n \circ h$ for all $g \in S^1$. A Borsuk–Ulam-type theorem for S^1-equivariant mappings implies that if Z is a finite-dimensional invariant subspace of X such that $\mathrm{Fix}\, S^1 \cap Z = \{0\}$ and D is an open bounded invariant neighborhood of 0 in Z, then S^1-ind$(\partial D) = (1/2)\dim Z$.

As the category of a Banach space $X = 1$, the classical Ljusternik–Schnirelman approach does not provide any information about the multiplicity of the unconstrained critical points of $f \in C^1(X, \mathbb{R})$. If f is invariant under the action on X of a compact group G and satisfies Palais–Smale condition, a Ljusternik–Schnirelman minimax method associated to a G-index provides multiplicity results for unconstrained critical points. Letting

$$\mathcal{A}_j = \{A \subset X : A \text{ is compact, invariant, and G-ind}(A) \geq j\}$$

$$c_j = \inf_{A \in \mathcal{A}_j} \sup_A f \quad (j = 1, 2, \ldots)$$

one shows as in classical Ljusternik–Schnirelman theory that if $c := c_j = c_{j+1} = \cdots = c_{j+q}$ for some j and some $q \geq 0$, then G-ind$(K_c) \geq q + 1$. The proof uses an equivariant deformation lemma.

$\mathbb{Z}^2$- and S^1-Invariant Functionals

In the case of the $\mathbb{Z}^2$-action, the following multiplicity result holds for possibly unbounded even $f \in C^1(X, \mathbb{R})$ satisfying the Palais–Smale condition and having the mountain pass geometry: if $Y \cap \{u \in X : f(u) \geq 0\}$ is bounded for each finite-dimensional subspace Y of X,

$f(0) = 0$, and $f(u) \geq a > 0$ on $\partial B(r)$, then f has infinitely many couples of critical points. As an application, the semilinear Dirichlet problem

$$\begin{aligned} \Delta u + \lambda u + |u|^{p-1} u = 0 \text{ in } \Omega \\ u = 0 \text{ on } \partial\Omega \end{aligned} \qquad [9]$$

has infinitely many solutions when $\Omega \subset \mathbb{R}^N$ is bounded, $1 < p < (N+2)/(N-2)$, and $\lambda < \lambda_1$, the smallest eigenvalue of $-\Delta$ with Dirichlet boundary conditions. The corresponding energy functional, defined on $W_0^{1,2}(\Omega)$ by

$$f(u) = \int_\Omega \left[\frac{\|\nabla u(x)\|^2}{2} - \lambda \frac{|u(x)|^2}{2} - \frac{|u(x)|^{p+1}}{p+1} \right] dx$$

satisfies the Palais–Smale condition. This condition fails in the critical case where $p = (N+2)/(N-2)$, at least at some levels c, and this lack of compactness creates both difficulties and interesting phenomena. This situation, which occurs in many important problems of geometry and physics (harmonic maps, Yang–Mills connections, Yamabe problem, equations of constant mean curvature, closed geodesics problems, etc.), reveals indeed, in physical terms, "phase transitions" or "particle creations" at the levels where the Palais–Smale condition fails. In the special case of eqn [9] with $p = (N+2)/(N-2)$, if $N \geq 4$, a positive solution exists when $\lambda \in [0, \lambda_1]$, and, if $N = 3$, the same is true for $\lambda \in [\lambda^*, \lambda_1]$ and some $\lambda^* \in [0, \lambda_1]$, with the optimal value $\lambda^* = \lambda_1/4$ when Ω is a ball. For $N \geq 4$, [9] has at least $\mathrm{cat}(\Omega)$ nontrivial solutions when $\lambda \in [0, \lambda^{**}]$ for some $\lambda^{**} < \lambda_1$. Such a lack of compactness, which can also occur for eqn [9] in $\mathbb{R}^N$ (nonlinear Schrödinger equation), is associated to the invariance of f with respect to the action of some noncompact group, coming, for example, from scale or gauge invariance. P L Lions' concentration–compactness method is useful to analyze those problems.

The following multiplicity theorem holds for an S^1-invariant $f \in C^1(X, R)$ satisfying Palais–Smale condition. Let $\mathrm{Fix}(S^1) = \{0\}$ and Z be a closed invariant vector subspace of X of positive finite dimension. If f is bounded from below, $f(u) \leq c < 0$ whenever $u \in Z$ and $\|u\| = r$, and $f(0) \geq 0$ for $u \in \mathrm{Fix}(S^1) \cap (f')^{-1}(0)$, then f has at least $\dim Z/2$ distinct S^1-orbits of critical points of f with critical values less or equal to c. This abstract theorem provides multiplicity results for the periodic solutions (closed orbits) of autonomous Hamiltonian systems in $\mathbb{R}^{2n}$

$$Ju' + \nabla H(u) = 0 \qquad [10]$$

where J is the symplectic matrix, $H \in C^1(\mathbb{R}^{2n}, \mathbb{R})$, and $c \in \mathbb{R}$ is such $\nabla H(u) \neq 0$ for $u \in H^{-1}(c)$. If $H^{-1}(c)$ bounds a strictly convex compact set C such that $B[r] \subset C \subset B[R]$ for some $0 < r < R < \sqrt{2}r$, then [10] has at least n closed orbits on $H^{-1}(c)$. The problem is reduced to finding the critical points of a suitable dual action functional acting on some space X of 2π-periodic functions having mean value zero. The S^1-action on X is defined by time translations $[\tau, u] \mapsto u_\tau = u(\cdot + \tau)$ for all $\gamma = e^{i\tau} \in S^1$. One takes, in the abstract result above, $Z = \{(\cos t)e + (\sin t)Je : e \in \mathbb{R}^{2n}\}$, so that $\dim Z = 2n$. The complete proof is quite involved, and, although some improvements of Ekeland–Lasry conditions have been obtained, the problem remains open to know if some pinching condition of the energy surface between spheres or ellipsoids is necessary.

Some Extensions

When dealing with unbounded functionals, it may be convenient to replace the Ljusternik–Schnirelman category $\mathrm{cat}_X(A)$ by a relative category $\mathrm{cat}_{X,Y}(A)$ with respect to a closed subset Y where, in the covering of A occurring in the classical definition, a set $A_0 \supset Y$ is added, which is continuously deformable in X into a subset of Y in such a way that points of Y remain in Y during the deformation. Clearly $\mathrm{cat}_{X,\emptyset}(A) = \mathrm{cat}_X(A)$. This allows us to prove, under some restrictions on the coefficients and the period, the existence of at least four periodic solutions for the double pendulum with periodic forcing of mean value zero. The classical Ljusternik–Schnirelman category gives at least three periodic solutions without restrictions, and the question of their necessity to obtain four solutions is open.

The relative category also gives a simpler proof of Conley–Zehnder's version of the Arnol'd conjecture (the existence of at least $2n+1$ geometrically distinct 1-periodic solutions for the Hamiltonian system

$$Ju' + \nabla H(t, u) = 0$$

with H 1-periodic in each variable), under minimal regularity assumptions upon H. The general conjecture, namely that the minimum number of fixed points of all Hamiltonian symplectomorphisms of a closed symplectic manifold M is larger than the minimum number of critical points of smooth functions f on M, remains open.

In another direction, a Ljusternik–Schnirelman theory for functionals defined on closed convex sets of a Banach space has been developed, which is specially well suited for the study of the Plateau problem for minimal surfaces, for surfaces of constant mean curvature, as well as for variational inequalities.

See also: Bifurcations of Periodic Orbits; Compact Groups and Their Representations; Floer Homology; Ginzburg–Landau Equation; Inequalities in Sobolev Spaces; Minimal Submanifolds; Minimax Principle in the Calculus of Variations; Saddle Point Problems; Sine-Gordon Equation; Spectral Theory for Linear Operators.

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Localization for Quasiperiodic Potentials

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Introduction

Discrete Schrödinger operators with quasiperiodic potentials are operators acting on $\ell^2(\mathbb{Z}^d)$ and defined by

$$H_\lambda = \Delta + \lambda V \qquad [1]$$

where Δ is the lattice tight-binding Laplacian

$$\Delta(n,m) = \begin{cases} 1, & \operatorname{dist}(n,m) = 1 \\ 0, & \text{otherwise} \end{cases}$$

and $V(n,m) = V_n\delta(n,m)$ is a potential given by $V_n = f(T_1^{n_1}\cdots T_d^{n_d}\theta), \theta \in \mathbb{T}^b$, where $T_i\theta = \theta + \omega_i$, and ω is an incommensurate vector. In certain cases Δ may also be replaced by a long-range Laplacian $L(n,m) = L(n-m)$ with $L(n) \to 0$ sufficiently fast. The questions of interest in the study of quasiperiodic and other ergodic operators are the nature and structure of the spectrum, behavior of the eigenfunctions, and the quantum dynamics: properties of the time evolution $\Psi_t = e^{itH}\Psi_0$ of an initially localized wave packet Ψ_0.

Of particular importance is the phenomenon of Anderson localization which is usually referred to the property of having pure point spectrum with exponentially decaying eigenfunctions. A stronger property of dynamical localization (see the section "Dynamical localization") indicates the insulator behavior, while ballistic transport, which for $d = 1$ follows from the absolutely continuous spectrum, indicates the metallic behavior.

Operators with ergodic potentials always have spectra (and pure point spectra, understood as closures of the set of eigenvalues) constant for a.c. realization of the potential. The individual eigenvalues however depend very sensitively on the phase. Moreover, the pure point spectrum of operators with ergodic potentials never contains isolated eigenvalues, so pure point spectrum in such models is dense in a certain closed set. An easy example of an operator with dense pure point spectrum is H_∞ which is operator [1] with $\lambda^{-1} = 0$, or pure diagonal. It has a complete set of eigenfunctions, characteristic functions of lattice points, with eigenvalues V_j. H_λ may be viewed as a perturbation of H_∞ for small λ^{-1}. However, since V_j are dense, small denominators $(V_i - V_j)^{-1}$ make any

perturbation theory difficult, for example, requiring intricate KAM-type schemes.

Various methods developed for the Anderson model (where V_n are i.i.d.r.v.'s) such as Fröhlich–Spencer multiscale analysis and its enhancements, or Aizenman–Molchanov method, do not work for quasiperiodic potentials as, among other reasons, quasiperiodicity does not allow for nice perturbations. The situation here is more difficult and the theory is far less developed than for the random case. With a few exceptions, the results are confined to the one-dimensional setting, and also the case of one frequency ($b=1$) has been much better understood than that of higher frequencies.

One might expect that H_λ with λ small can be treated as a perturbation of $H_0=\Delta$, and therefore have absolutely continuous spectrum. It is not the case though for random potentials in $d=1$, where Anderson localization holds for all λ. The same is expected for random potentials in $d=2$ (but not higher). Moreover, in one-dimensional case, there is strong evidence (numerical, analytical, as well as rigorous) that even models with very mild stochasticity in the underlying dynamics (and sufficiently nice sampling functions) have point spectrum for all values of λ, like in the random case (e.g., $V_n=\lambda f(n^\sigma\alpha+\theta)$, for any $\sigma>1$). At the same time, for quasiperiodic potentials, one can in many cases show absolutely continuous spectrum for λ small as well as pure point spectrum for λ large (see below), and therefore there is a metal–insulator transition in the coupling constant. It is an interesting question whether quasiperiodic potentials are the only ones with metal–insulator transition in 1D.

Perturbative and Nonperturbative Approaches

It is probably fair to say that much of the theory of qusiperiodic operators has been first developed around the almost-Mathieu operator, which is

$$H_{\lambda,\omega,\theta}=\Delta+\lambda f(\theta+n\omega) \qquad [2]$$

acting on $\ell^2(\mathbb{Z})$, with $f:\mathbb{T}\to\mathbb{T}; f(\theta)=\cos(2\pi\theta)$. Several KAM-type approaches, starting with the pioneering work of Dinaburg–Sinai in 1975, were developed, in 1980s and 1990s, for this or similar models in both large and small coupling regimes. Of those, the most robust and detailed is the reducibility result of Eliasson (1998) that settled the case of small couplings for sufficiently regular potentials.

The common feature of those perturbative approaches is that, besides all of them being rather intricate multistep procedures, they rely extensively on eigenvalue and eigenfunction parametrization and perturbation arguments.

The common feature of the perturbative results in the quasiperiodic setting is that they typically provide no explicit estimates on how large (or small) the parameter λ should be, and, more importantly, λ clearly depends on ω at least through the constants in the Diophantine characterization of ω.

In contrast, the nonperturbative results allow effective (in many cases even optimal) and, most importantly, independent of ω, estimates on λ. The latter property (uniform in ω estimates on λ) has been often taken as a definition of a nonperturbative result.

Recently developed nonperturbative methods are also quite different from the perturbative ones in that they do not employ multiscale schemes: usually only a few (from one to three) sufficiently large scales are involved, do not use the eigenvalue parametrization, and rely instead on direct estimates of the Green's function. They are also significantly less involved, technically. One may think that in these latter respects they resemble the Aizenman–Molchanov method for random localization. It is, however, a superficial similarity, as, on the technical side, they are still closer to and do borrow certain ideas from the multiscale analysis proofs of localization.

Lyapunov Exponents

Here for simplicity we consider the quasiperiodic case, although the definition of the Lyapunov exponents and some of the mentioned facts apply more generally to the one-dimensional ergodic case.

Let $d=1$. For an energy $E\in\mathbb{R}$ the Lyapunov exponent $\gamma(E)$ is defined as

$$\gamma(E)=\lim_{n\to\infty}\frac{\int_0^1\ln\|M_k(\theta,E)\|\,d\theta}{k} \qquad [3]$$

where

$$M_k(\theta,E)=\prod_{n=k-1}^{0}\begin{pmatrix}E-\lambda f(\omega n+\theta) & -1\\ 1 & 0\end{pmatrix}$$

is the k-step transfer matrix for the eigenvalue equation $H\Psi=E\Psi$.

In physics literature, positivity of the Lyapunov exponent is often taken as an implicit definition of localization, as Lyapunov exponent is often called the inverse localization length. Thus, we will be interested in the regime when Lyapunov exponents are positive for all energies in a certain interval intersecting the spectrum. If this condition holds for all $E\in\mathbb{R}$, there is no absolutely continuous

component in the spectrum for all θ. Positivity of Lyapunov exponents, however, does not imply localization or exponential decay of eigenfunctions (in particular, neither for the Liouville ω nor for the resonant $\theta \in \mathbb{T}^b$).

Nonperturbative methods, at least in their original form, stem to a large extent from estimates involving the Lyapunov exponents and exploiting their positivity.

The general theme of the results on positivity of $\gamma(E)$, as suggested by perturbation arguments, is that the Lyapunov exponents are positive for large λ. This subject has had a rich history. The strongest result in this general context up to date is the following theorem (Bourgain 2003):

Theorem 1 *Let f be a nonconstant real-analytic function on $\mathbb{T}^b$, and H given by* [1]. *then, for $\lambda > \lambda(f)$, we have $\gamma(E) > (1/2) \ln \lambda$ for all E and all incommensurate vectors ω.*

Corollaries of Positive Lyapunov Exponents

The almost-Mathieu operator On one hand the almost-Mathieu operator, while simple looking, seems to represent most of the nontrivial properties expected to be encountered in the more general case. On the other hand it has a very special feature: the duality (essentially a Fourier) transform maps H_λ to $H_{4/\lambda}$; hence $\lambda = 2$ is the self-dual point. Aubry and Andre in 1980, conjectured that for this model, for irrational ω a sharp metal–insulator transition in the coupling constant λ occurs at the critical value of coupling $\lambda = 2$: the spectrum is pure point for $\lambda > 2$ and purely absolutely continuous for $\lambda < 2$. This conjecture was modified based on later discoveries of singular-continuous spectrum in this context for frequencies or phases with certain arithmetic properties. The modified conjecture stated pure point spectrum for Diophantine ω and a.e. θ for $\lambda > 2$ and pure absolutely continuous spectrum for $\lambda < 2$ for all ω,θ. The spectrum at $\lambda = 2$ is singular continuous for all ω and a.e. θ(this follows from a combination of works by Gordon, Jitomirskaya, Last, Simon Avila, and Krikoryan).

As with the KAM methods, the almost-Mathieu operator was the first model where the positivity of Lyapunov exponents was effectively exploited (Jitomirskaya 1999):

Theorem 2 *Suppose ω is Diophantine and $\gamma(E,\omega) > 0$ for all $E \in [E_1, E_2]$. Then the almost-Mathieu operator has Anderson localization in $[E_1, E_2]$ for a.e. θ.*

The condition on θ can be made explicit (arithmetic) and close to optimal. This, combined with the mentioned results on the Lyapunov exponents, critical value $\lambda = 2$, and duality, gives the following description in the Diophantine case:

Corollary 3 *The almost-Mathieu operator $H_{\omega,\lambda,\theta}$ has*

1° *for $\lambda > 2$, Diophantine $\omega \in \mathbb{R}$ and almost every $\theta \in \mathbb{R}$, only pure point spectrum with exponentially decaying eigenfunctions.*

2° *for $\lambda = 2$, all $\omega \notin \mathbb{Q}$, and a.e. $\theta \in \mathbb{R}$ purely singular-continuous spectrum.*

3° *for $\lambda < 2$, Diophantine $\omega \in \mathbb{R}$ and a.e. $\theta \in \mathbb{R}$, purely absolutely continuous spectrum.*

Precise arithmetic descriptions of ω, θ are available. Thus, the Aubry–Andre conjecture is settled at least for almost all ω, θ. One should mention, however, that while 1° can be made optimal by existing methods, both 2° and 3° are expected to hold for all θ and all $\omega \notin \mathbb{Q}$, and such extension remains a challenging problem (see Simon (2000)).

The method in the above work, while so far the only nonperturbative method available allowing precise arithmetic conditions, uses some specific properties of the cosine. It extends to certain other situations, for example, quasiperiodic operators arising from Bloch electrons in a perpendicular magnetic field, where the lattice is triangular or has next-nearest-neighbor interactions. However, it does not extend easily to the multifrequency or even general analytic potentials. A much more robust method was developed by Bourgain–Goldstein (2000), which allowed them to extend (a measure-theoretic version of) the above localization result to the general real analytic as well as the multi-frequency case. Note that essentially no results were previously available for the multifrequency case, even perturbative.

Theorem 4 *Let f be nonconstant real analytic on $\mathbb{T}^b$ and H given by* [2]. *Suppose $\gamma(E,\omega) > 0$ for all $E \in [E_1, E_2]$ and a.e. $\omega \in \mathbb{T}^b$. Then for any θ, H has Anderson localization in $[E_1, E_2]$ for a.e. ω.*

Combining this with Theorem 1, Bourgain (2003) obtained that for $\lambda > \lambda(f)$, H as above satisfies Anderson localization for a.e. ω. Those results were recently extended by S Klein to potentials belonging to certain Gevrey classes. One very important ingredient of this method is the theory of semialgebraic sets that allows one to obtain polynomial algebraic complexity bounds for certain "exceptional" sets. Combined with measure estimates coming from the large deviation analysis of $(1/n) \ln \|M_n(\theta)\|$ (using subharmonic function theory and involving approximate Lyapunov exponents),

this theory provides necessary information on the geometric structure of those exceptional sets. Such algebraic complexity bounds also exist for the almost-Mathieu operator and are actually sharp albeit trivial in this case due to the specific nature of the cosine.

Further corollaries of positive Lyapunov exponents for analytic sampling functions f and $b=1$ include Hölder regularity of the integrated density of states, zero-dimensionality of spectral measures for all ω, θ, almost Lipshitz continuity of spectral gaps, continuity of measure of the spectrum (in frequency), and vanishing of lower transport exponents for all ω, θ. Some weaker statements are available for $b>1$ or f belonging to certain Gevrey classes.

Without Lyapunov Exponents

While having led to significant advances, Lyapunov exponents have obvious limitations, as any method based on them is restricted to one-dimensional nearest-neighbor Laplacians. It turns out that the above methods can be extended to obtain nonperturbative results in certain quasi-one-dimensional situations where Lyapunov exponents do not exist. For example, nonperturbative localization results extend to the strip (of arbitrary dimension).

The following nonperturbative theorem deals with the case of small coupling:

Theorem 5 *Let H be an operator* [2], *where f is real analytic on $\mathbb{T}$ and ω is Diophantine. then, for $\lambda < \lambda(f)$, H has purely absolutely continuous spectrum for a.e. θ.*

We note that an analog of this theorem does not hold in the multifrequency case (see next section). The results of this type are obtained by a method (developed by Bourgain and Jitomirskaya in 2000–02) that studies large deviations for the quantities of the form $(1/n)\ln|\det(H-E)_\Lambda|$ and path-determinant expansion for the matrix elements of the resolvent. Those techniques apply also to certain other situations with long-range Laplacians, for example, the kicked-rotor model. Theorem 5 is a result on nonperturbative localization in disguise as it was obtained using duality from a localization theorem for a dual model which has in general a long-range Laplacian and a cosine potential, and was in turn obtained by an extension of the method of Jitomirskaya (1999). A certain measure-theoretic version of it allowing nonlocal Laplacians but leading only to continuous spectrum is also available (see Bourgain (2004)).

Multidimensional Case: $d>1$

As mentioned above, there are very few results in the multidimensional lattice case ($d>1$). Essentially, the only result that existed before the recent developments was a perturbative theorem – an extension by Chulaevsky–Dinaburg of Sinai's method to the case of operator [1] on $\ell^2(\mathbb{Z}^d)$ with $V_n=\lambda f(n\cdot\omega), \omega\in\mathbb{R}^d$, where f is a cos-type function on $\mathbb{T}$. This also holds nonperturbatively for any real-analytic f (see Bourgain (2004)). Note that since $b=1$, this avoids most serious difficulties and is therefore significantly simpler than the general multidimensional case. We therefore have:

Theorem 6 *For any $\epsilon>0$ there is $\lambda(f,\epsilon)$, and, for $\lambda>\lambda(f,\epsilon), \Omega(\lambda,f)\subset\mathbb{T}^d$ with $\mathrm{mes}(\Omega)<\epsilon$, so that for $\omega\notin\Omega$, operator* [1] *with V_n as above has Anderson localization.*

This should be confronted with the following theorem of Bourgain:

Theorem 7 *Let $d=2$ and $f(\theta)=\cos 2\pi\theta$ in $H=H_\omega$ defined as above. Then for any λ measure of ω s.t. H_ω has some continuous spectrum is positive.*

Therefore, for large λ there will be both ω with complete localization as well as those with at least some continuous spectrum. This shows that nonperturbative results do not hold in general in the multidimensional case! Perturbative results, however, had been obtained, see next section.

A similar (in fact, dual) situation is observed for one-dimensional multifrequency ($d=1; b>1$) case at small disorder. One has, by duality:

Theorem 8 *Let H be given by* [2] *with $\theta,\omega\in\mathbb{T}^b$ and f real analytic on $\mathbb{T}^b$. Then for any $\epsilon>0$ there is $\lambda(f,\epsilon)$ s.t. for $\lambda<\lambda(f,\epsilon)$ there is $\Omega(\lambda,f)\subset\mathbb{T}^b$ with $\mathrm{mes}(\Omega)<\epsilon$ so that for $\omega\notin\Omega$, H has purely absolutely continuous spectrum.*

And also

Theorem 9 *Let $d=1, b=2$ and f be a trigonometric polynomial on $\mathbb{T}^2$ with a nondegenerate maximum. Then for any λ, measure of ω s.t. H_ω has some point spectrum, dense in a set of positive measure, is positive.*

Therefore, unlike the $b=1$ case (see Theorem 5), nonperturbative results do not hold for absolutely continuous spectrum at small disorder.

Perturbative Localization by Nonperturbative Methods

While the above demonstrates the limitations of the nonperturbative results, the nonperturbative

methods have been applied to significantly simplify the proofs and obtain new perturbative results that previously had been completely beyond reach.

Many such applications, that are outside the scope of this article, are described in Bourgain (2004). In particular, new results on the construction of quasiperiodic solutions in Melnikov problems and nonlinear PDEs, obtained by using certain ideas developed for nonperturbative quasiperiodic localization (e.g., the theory of semialgebraic sets), are presented there. Other results in this group contain localization for the skew-shift model by Bourgain–Goldstein–Schlag, almost periodicity for the quantum kicked-rotor model by Bourgain and Bourgain–Jitomirskaya, and localization for potentials in higher Gevrey classes by S Klein.

The main goal in a nonperturbative method is to obtain exponential off-diagonal decay for the matrix elements of the Green's function of box-restricted operators along with subexponential bounds on the distance from the spectrum of such box restrictions to a given energy. From that result one can obtain localization through elimination of energy via an argument involving complexity bounds on semialgebraic sets (see Bourgain (2004)).

A nonperturbative way to achieve the desired Green's function estimates uses Cramer's rule to represent the matrix elements of the resolvent. Then, in the one-dimensional (in space) case it is often possible to obtain the estimates from the positivity of Lyapunov exponents: uniformly for the numerator, and from large deviation bounds for the subharmonic functions for the denominator. This is done in one step for a sufficiently large scale (see the subsection "Corollaries of positive Lyapunov exponents")

A perturbative way consists of establishing the desired estimates in a multiscale scheme: namely, the estimates are proved outside a set of parameters of (subexponentially) decaying (in the size of the box) measure. Moreover, this set should be shown to have a semialgebraic description, in order to make possible sublinear upper bounds on the number of times a trajectory of a given phase (under the underlying rotation or other ergodic transformation of the torus) hits the "forbidden" set. This, plus certain subharmonic function arguments, allows passage to a larger scale through a repeated use of the resolvent identity.

An application that is most relevant to the current article is localization for a "true" $d>1$ situation. The best currently available result is the following very recent theorem (Bourgain 2005):

Theorem 10 *Let $d=b$ and let f be real analytic on $\mathbb{T}^d$ such that for all $i=1,\ldots,d$ and $(\theta_1,\ldots,\theta_{i-1},\theta_{i+1},\ldots,\theta_d)\in\mathbb{T}^{d-1}$, the map*

$$\theta_i \mapsto v(\theta_1,\ldots,\theta_i,\ldots,\theta_d)$$

is a nonconstant function of $\theta_i\in\mathbb{T}$. Then for any $\epsilon>0$ there is $\lambda(f,\epsilon)$ s.t. for $\lambda>\lambda(f,\epsilon)$ there is $\Omega(\lambda,f)\subset\mathbb{T}^d$ with $\mathrm{mes}(\Omega)<\epsilon$ so that for $\omega\notin\Omega$ operator [1] with $V_n=\lambda f(n_1\omega_1,n_2\omega_2)$ has Anderson (and dynamical) localization.

This result was obtained previously, for $d=2$ only, by Bourgain, Goldstein, and Schlag. There were some serious purely arithmetic difficulties that prevented an extension of this result to higher dimensions. In the previous results on localization there were two major steps: estimations on the Green's function for fixed energy and elimination of energy. The main difficulty in the multidimensional case lies in establishing the sublinear bound described above, that enters in the first step. It is for this bound that an arithmetic condition on ω was needed. The condition used was to guarantee that the number of $(n_1,n_2)\in[1,N]^2$ such that $(n_1\omega_1, n_2\omega_2)(\mathrm{mod}\,\mathbb{Z}^2)\in S$ is bounded from above by N^α for some $\alpha<1$, uniformly for all semialgebraic sets S of degree D, with $D'/D=o(1/N)$ and with the measure of all horizontal and vertical sections S_x satisfying $\log\mathrm{mes}S_x=o(\log 1/N)$. This condition roughly means that too many points close to an algebraic curve of a bounded degree would force it to oscillate more than it should. Such a statement is essentially two dimensional and not extendable to $d\geq 3$. In Theorem 10, Bourgain circumvents it by using from the beginning the theory of semialgebraic sets to eliminate energy and the translation variable to get conditions on ω (that depend on the potential) already in the first step.

Dynamical Localization

Anderson localization does not in itself guarantee absence of quantum transport, or nonspread of an initially localized wave packet, as characterized, for example, by boundedness in time of moments of the position operator. This was first observed in del Rio *et al.* (1996), where a rather artificial example of coexistence of exponential localization and quantum transport was constructed. However, such phenomena also happen in models of interest to physicists such as the random dimer model. Considering for simplicity the second moment

$$\langle x^2\rangle_T=\frac{1}{T}\int_0^T\sum_n|\Psi_t(n)|^2n^2\,dt$$

we will say that H exhibits dynamical localization if $\langle x^2\rangle_T<\text{const.}$ We will say that the family $\{H_\theta\}_{\theta\in\mathbb{T}^b}$ exhibits strong dynamical localization if $\int_{\mathbb{T}^b}d\theta\,\sup_t\langle x^2\rangle_t<\text{const.}$ We note that the results mentioned below will hold with more restrictive

definitions of dynamical localization (involving the higher moments of the position operator) as well. Dynamical localization implies pure point spectrum by RAGE theorem so it is a strictly stronger notion.

It turns out that nonperturbative methods allow for such dynamical upgrades as well. For the almost-Mathieu operator, strong dynamical localization holds throughout the regime of localization. It was shown by Bourgain and Jitomirskaya that in Theorems 4 and 6 as well as some other localization results, dynamical localization also holds (see Bourgain (2004)). However, methods that require elimination of certain frequencies based on implicit conditions currently do not provide sufficient information to obtain strong (i.e., averaged) dynamical localization, like what was done in the almost-Mathieu case.

Quasiperiodic Localization and Cantor Spectrum

A remarkable feature of quasiperiodic operators with $b=d=1$ is their tendency to have Cantor spectrum. In particular, it was conjectured that all almost-Mathieu operators (for all nonzero couplings and all irrational frequencies) have Cantor spectrum. This conjecture became known as the Ten Martini problem. In a significant recent development (Puig 2004), it was shown that for Diophantine frequencies Cantor structure of the spectrum follows from localization for phase $\theta=0$, with corresponding eigenvalues being the boundaries of noncollapsed gaps. The key idea here is that for energies dual to eigenvalues of H_0, corresponding to localized eigenfunctions, the rotation number of the transfer-matrix cocycle is of the form $k\omega(\mathrm{mod}\mathbb{Z})$, thus they are the ends of the gaps (possibly collapsed). However, a collapsed gap in this case would correspond to reducibility of the system to the identity which can be shown to contradict the simplicity of pure point spectrum for the dual model. Since those energies form a dense subset of the spectrum the result follows. The same idea works, thus establishing Cantor spectrum, for potentials that are generic in certain sense. Localization also played an important role in the final proof of the Ten Martini conjecture, for all irrationals (Avila and Jitomirskaya 2005). It can be shown that proving localization for a large set of phases allows one to conclude reducibility of the transfer-matrix cocycle for the dual model, for a large set of energies, and this in turn can be shown to contradict the presence of an interval in the spectrum.

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See also: Multiscale Approaches; Quantum Hall Effect; Quasiperiodic Systems; Schrödinger Operators; Stability Theory and KAM.

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Loop Quantum Gravity

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Introduction

Loop quantum gravity (LQG) is a mathematical formalism that defines a tentative quantum theory of spacetime. Equally, the formalism provides a description of the gravitational field in regimes in which its quantum properties cannot be neglected. The distinctive feature of LQG is to be a quantum field theory consistent with general relativity.

According to general relativity, the physical fields that form the world do not live on a background spacetime. Rather, these fields make up spacetime themselves ("background independence"). Accordingly, the quanta of a quantum field theory compatible with this principle – the *s*-knots described below – do not live on a background spacetime: rather, they themselves form physical spacetime.

This physical idea is realized in the formalism by the gauge invariance under active diffeomorphisms of the manifold on which the fields are originally defined ("diffeomorphism invariance"). Such gauge invariance renders the localization of the field's excitations on the manifold physically irrelevant.

LQG implements these physical motivations by merging two traditional lines of thinking in theoretical physics. The first is the long-standing idea that gauge fields are naturally understood in terms of variables associated to lines (holonomies of the gauge connection, Wilson loops, Faraday lines, ...). This idea can be traced to Faraday's initial intuition that gave birth to modern field theory: physical fields are real entities formed by lines. The second is the background-independent canonical or covariant quantization of general relativity developed by following the ideas of Wheeler, DeWitt, and Hawking. Each of these two lines of research has encountered serious obstructions, but the two turn out to solve each others' difficulties: the formulation in terms of holonomies renders the old ill-defined background-independent quantum gravity well defined; conversely, background independence cures the divergences associated to the Wilson loop basis.

The formalism of LQG can be separated into two parts. A kinematics, describing the quantum properties of space, and a dynamics, describing its evolution. Here we outline the LQG kinematics, and we give only the main result of the LQG dynamics.

LQG can be extended to include standard matter couplings such as fermions and Yang–Mills fields. It finds numerous applications, for instance, in early cosmology, astrophysics and black hole thermodynamics (*see* Black Hole Mechanics, Quantum Cosmology).

So far no empirical evidence supports the physical correctness of this – nor of any other – tentative theory of quantum gravity.

General Relativity in Canonical Form

Classical general relativity is the field theory describing the gravitational field and the structure of physical spacetime. It is a well-established physical theory, strongly supported empirically.

In its Riemannian version, the theory can be written in canonical form in terms of two fields on a three-dimensional (3D) manifold Σ with coordinates $x^a (a = 1, 2, 3)$: a 2-form $E = E^a \epsilon_{abc}\, dx^a\, dx^b$, called the "triad field" and a 1-form $A = A_a\, dx^a$, called the "gravitational connection" (ϵ_{abc} is the totally antisymmetric tensor density). Both take values in the su(2) algebra, and they satisfy the three "constraint" equations

$$\mathcal{G} = D_a E^a = 0 \quad [1]$$

$$C_a = \mathrm{tr}[F_{ab} E^a] = 0 \quad [2]$$

$$C = \mathrm{tr}[F_{ab} E^a E^b] = 0 \quad [3]$$

D_a is the SU(2) covariant derivative defined by the connection A, F_{ab} is the SU(2) curvature of A, and the trace is on su(2).

E and A are canonically conjugate: their Poisson brackets are $\{E^a(x), A_b(y)\} = 8\pi G c^{-3} \delta^a_b \delta^3(x, y)$; where G is the Newton constant, c is the speed of light, δ^a_b is the Kronecker delta, and $\delta^3(x, y)$ is the Dirac-delta on Σ, which is a scalar density in x. The Poisson brackets of $\mathcal{G}$ with the fields define their SU(2) gauge transformations: E transforms in the adjoint representation and A transforms as a connection. The Poisson brackets of C_a (more precisely, of an appropriate linear combination of C_a and $\mathcal{G}$) with the fields determine their transformation under a diffeomorphism of Σ: E transforms as a 2-form and A as a 1-form. The Poisson brackets of C with the fields generate their coordinate time evolution. If the t derivatives of the fields $E(x^a, t)$ and $A(x^a, t)$ are given by their Poisson brackets with (the 3D integral of) C, then (assuming that the determinant $E = \sqrt{\det \mathrm{tr}[E^a E^b]}$ does not vanish) the metric field

$g^{00}=1$, $g^{a0}=0$, $g^{ab}=\mathrm{tr}[E^aE^b]/E$ is a general solution of the Riemannian Einstein equations in a fixed gauge.

The physical Lorentzian theory can be obtained in this formalism in two ways. Either by adding an appropriate term to eqn [3], or by taking A in sl(2,C) and satisfying a suitable reality condition. (For more details, *see* Canonical General Relativity.)

Spin Network and *s*-Knot States

LQG can be defined as a Schrödinger quantization of the canonical formalism described above. The space of the quantum states is defined as a Hilbert space $\mathcal{K}$ of Schrödinger wave functionals $\Psi[A]$ of the gravitational connection. The nontrivial aspect of this construction is the definition of a scalar product invariant under the two kinematical gauge invariances of the theory: the local SU(2) and the diffeomorphisms transformations generated by the constraints [1] and [2]. The state space $\mathcal{K}$ is defined as follows (*see* Quantum Geometry and its Applications for an essentially equivalent construction).

Given an su(2) connection A and an oriented path $\gamma : s \in [0,1] \to x^a(s) \in \Sigma$, recall that the "holonomy" $U[A,\gamma]$ of A along γ is the element of SU(2) defined by

$$\frac{\mathrm{d}}{\mathrm{d}s}U[A,\gamma](s)+\dot{\gamma}^a(s)A_a(\gamma(s))U[A,\gamma](s)=0 \quad [4]$$

$$U[A,\gamma](0)=\mathbb{1}, \qquad U[A,\gamma]=U[A,\gamma](1) \quad [5]$$

where $\dot{\gamma}^a(s)\equiv \mathrm{d}x^a(s)/\mathrm{d}s$ is the tangent to the path. The solution of this equation is usually written in the form

$$U[A,\gamma]=\mathcal{P}\mathrm{e}^{\int_\gamma A} \quad [6]$$

where the path ordered $\mathcal{P}$ is understood as acting on the power series expansion of the exponential.

Let $\mathcal{A}$ be the space of the smooth connections A on Σ. (For technical reasons, it is convenient to consider smooth fields A defined everywhere in Σ except at most at a finite number of points, and the group $Diff^*$ of the "extended diffeomorphisms" defined by the continuous invertible maps $\phi:\Sigma\to\Sigma$ that are smooth everywhere in Σ except at most at a finite number of points.) A graph Γ is an ordered collection of smooth oriented paths, γ_l, denoted as links, with $l=1,\ldots,L$, where the links overlap only at their endpoints, called nodes. Given a graph Γ and a smooth, Haar-integrable complex function $f:U\in(\mathrm{SU}(2))^L\mapsto f(U)\in C$, the couple (Γ,f) defines the ("cylindrical") functional of A

$$\Psi_{\Gamma,f}[A]=f(U[A,\Gamma]) \quad [7]$$

$$U[A,\Gamma]\equiv(U[A,\gamma_1],\ldots,U[A,\gamma_L]) \quad [8]$$

Let $\mathcal{L}$ be the linear space of all functionals $\Psi_{\Gamma,f}[A]$, for all Γ and f. $\mathcal{L}$ is dense (in an appropriate sense) in the space of all continuous functionals on $\mathcal{A}$.

An SU(2) and $Diff^*$ invariant scalar product can be defined in $\mathcal{L}$ as follows. If two functionals $\Psi_{\Gamma,f}[A]$ and $\Psi_{\Gamma,g}[A]$ are defined by the same graph Γ, define

$$\langle\Psi_{\Gamma,f}|\Psi_{\Gamma,g}\rangle\equiv\int \mathrm{d}U\,\overline{f(U)}\,g(U) \quad [9]$$

where $\mathrm{d}U$ is the Haar measure on $(\mathrm{SU}(2))^L$. The extension to functionals defined on different graphs is obtained by observing that (Γ,f) and (Γ',f') define the same functional if Γ contains Γ' and f is independent of the variables in Γ but not in Γ'. It follows that any two given functionals $\Psi_{\Gamma',f'}$ and $\Psi_{\Gamma'',g''}$ can be written as functionals $\Psi_{\Gamma,f}$ and $\Psi_{\Gamma,g}$ with the same graph Γ, where Γ is obtained from the union of Γ' and Γ''. Using this, the scalar product [9] is defined for any two functionals in $\mathcal{L}$:

$$\langle\Psi_{\Gamma',f'}|\Psi_{\Gamma'',g''}\rangle\equiv\langle\Psi_{\Gamma,f}|\,\Psi_{\Gamma,g}\rangle \quad [10]$$

Standard completion in the Hilbert norm defines the kinematical Hilbert space $\mathcal{K}$ of LQG. $\mathcal{L}$ is dense in $\mathcal{K}$ and defines the Gelfand triple $\mathcal{L}\subset\mathcal{K}\subset\mathcal{L}^*$. $\mathcal{K}$ carries a natural unitary representation of the group of local SU(2) representations and a natural unitary representation U_ϕ of the group of the extended diffeomorphism of Σ. These two properties are nontrivial; they represent the main physical motivation for the definition of the scalar product. The SU(2)-invariant subspace of $\mathcal{K}$ is a proper subspace $\mathcal{K}_0$.

An orthonormal basis in $\mathcal{K}_0$ can be defined using the Peter–Weyl theorem. The basis states are labeled by a graph Γ, by the assignment of a nonvanishing spin j_γ to each link $\gamma\in\Gamma$ and by the assignment of a basis element i_n in the space of the intertwiners (invariant tensors in the tensor product of the representations space of the adjacent links) at each node n of Γ. The triple $S=(\Gamma,j_\gamma,i_n)$ is called an imbedded *spin network*. The quantum state $\Psi_S[A]=\langle A|S\rangle$ in $\mathcal{K}_0$ labeled by the spin network $S=(\Gamma,j_\gamma,i_n)$ is the cylindrical function obtained by contracting the representation matrices of the holonomies $U(A,\gamma)$, in the representations j_γ, with the invariant tensors at the nodes.

The diffeomorphism-invariant state space $\mathcal{K}_{\mathrm{diff}}$ is the SU(2) and diffeomorphism invariant subspace of $\mathcal{L}^*$. It is the (closure of the) image of the map $P_{\mathrm{diff}}:\mathcal{L}\to\mathcal{L}^*$ defined by

$$(P_{\mathrm{diff}}\Psi)(\Psi')=\sum_{\Psi''=U_\phi\Psi}\langle\Psi'',\Psi'\rangle \quad \forall\Psi,\Psi'\in\mathcal{K} \quad [11]$$

The sum is over all states Ψ'' in $\mathcal{L}$ for which there exists a diffeomorphism ϕ such that $\Psi'' = U_\phi \Psi$; this is a finite sum. The scalar product on this image is naturally defined by

$$\langle P_{\text{diff}}\Psi_S, P_{\text{diff}}\Psi_{S'}\rangle_{\mathcal{K}_{\text{diff}}} \equiv (P_{\text{diff}}\Psi_S)(\Psi_{S'}) \qquad [12]$$

The space $\mathcal{K}_{\text{diff}}$ obtained in this manner is separable.

The images $|s\rangle = P_{\text{diff}}|S\rangle$ of the spin network states are called s-knot states. They span $\mathcal{K}_{\text{diff}}$. They are determined only by the diffeomorphism equivalence class s of the spin network S. Namely, by an abstract (non-imbedded) knotted graph, colored with spins and intertwiners. These colored knots are called s-knots or abstract spin networks. The s-knot states have a straightforward physical interpretation as quantum excitations of space, discussed below.

Operators and Quanta of Space

The state space defined above carries a quantum representation of classical observables of general relativity. The classical quantity $U[A, \gamma]$, a function of the field variable A, acts naturally as a multiplicative operator on $\mathcal{K}$. Thus, $\mathcal{K}$ provides a Schrödinger functional representation $\Psi[A]$ of quantum gravity, which diagonalizes the (holonomy of the) gravitational connection. The two constraints [1] and [2] generate SU(2) gauge and diffeomorphism transformations on A. The corresponding transformations on the Schrödinger functional states $\Psi[A]$ are given by the unitary representations mentioned above. The quantum implementation of the two constraint equations [1] and [2], following Dirac's theory of constrained quantum systems, is the requirement of invariance under these transformations. The space $\mathcal{K}_{\text{diff}}$ is the solution to these requirement.

The triad field operator E can be defined only if suitably smeared. Since E is a 2-form, its geometrically natural smearing is with a 2D surface. (The 1-form field A is smeared over a line in $U[A, \gamma]$.) Given a finite 2D surface $\mathcal{S} : \sigma = (\sigma^1, \sigma^2) \mapsto x^a(\sigma) \in \Sigma$, the smeared field

$$E[\mathcal{S}] = \int_{\mathcal{S}} E = \int \mathrm{d}^2\sigma\, \epsilon_{abc} \frac{\partial x^a}{\partial \sigma^1} \frac{\partial x^b}{\partial \sigma^2} E^c(x(\sigma)) \qquad [13]$$

is quantized by the functional derivative operator

$$E[\mathcal{S}] \equiv -\mathrm{i}\hbar \frac{8\pi G}{c^3} \int \mathrm{d}^2\sigma\, \epsilon_{abc} \frac{\partial x^a}{\partial \sigma^1} \frac{\partial x^b}{\partial \sigma^2} \frac{\delta}{\delta A_c(x(\sigma))} \qquad [14]$$

This operator is well defined on $\mathcal{K}$ and the quantum operators $E[\mathcal{S}]$ and $U[A, \gamma]$ define a linear representation of the Poisson algebra of the corresponding classical quantities. Thus, they define a quantization of the kinematics of general relativity. Notice that in a general covariant quantum field theory field operators can be well defined even if smeared on low-dimensional regions, while in conventional quantum field theory, these operators need to be smeared over 3D or 4D regions.

A simple calculation shows that if $\mathcal{S}$ and γ intersect once,

$$E_v[\mathcal{S}]U[A, \gamma] = \pm \mathrm{i}\hbar \frac{8\pi G}{c^3} U[A, \gamma_1] v U[A, \gamma_2] \qquad [15]$$

where $v \in \mathrm{su}(2)$, we have written $E_v = \mathrm{tr}[vE]$, $\gamma_{1,2}$ are the two paths into which γ is partitioned by the surface, and the sign is determined by the relative orientation of $\mathcal{S}$ and γ. More generally, $E[\mathcal{S}]U[A, \gamma]$ is a sum of one such term per intersection between $\mathcal{S}$ and γ.

Composite operators can be constructed in terms of these operators. In particular, using standard formulas in classical general relativity, the area of the surface $\mathcal{S}$ can be written as a Riemann sum

$$A[\mathcal{S}] = \lim_{N \to \infty} \sum_n \sqrt{\mathrm{tr}[E(\mathcal{S}_n)E(\mathcal{S}_n)]} \qquad [16]$$

where $\mathcal{S}_n, n = 1, \ldots, N$, is a Riemann partition of the surface. A straightforward calculation based on eqn [15] shows that, if $\mathcal{S}$ cuts n links of a spin network carrying spins $(j_1 \ldots j_n) = \boldsymbol{j}$, then the spin network state $|S\rangle$ is an eigenstate of $A[\mathcal{S}]$ with eigenvalue

$$A_{\boldsymbol{j}} = \frac{8\pi \hbar G}{c^3} \sum_{i=1,n} \sqrt{j_i(j_i + 1)} \qquad [17]$$

where $j_i = 1/2, 1, 3/2, 2, \ldots$ These are therefore discrete eigenvalues of the area. All eigenvalues of the area operator $A[\mathcal{S}]$ are real and discrete and $A[\mathcal{S}]$ is a self-adjoint operator. Similar results are obtained for the volume operator. This gets a discrete contribution for each node of a spin network.

These spectral properties of the area and volume operators determine the physical interpretation of the spin network states: the nodes of the spin network represent quanta of space with quantized volume; the nodes are connected by links representing quanta of surface with quantized area. The graph Γ determines the adjacency relations between the individual quanta of space; the intertwiners i_n are volume quantum numbers; the spins j_γ are area quantum numbers.

The interpretation carries over to the s-nodes, which represent the same quantum excitations of space, up to its manifold coordinatization, which is physically irrelevant because of the gauge invariance under

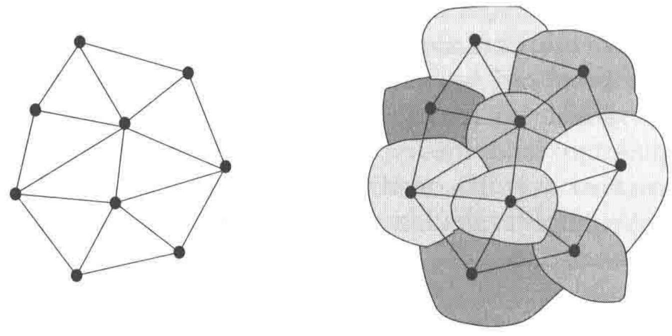


Figure 1 The graph of an s-knot, namely an abstract spinfoam, and the set of quanta of space it represents. Each node n of the graph defines a quantum of space. The associated intertwiner i_n is the corresponding volume quantum number. Two quanta of space are adjacent if the corresponding nodes are linked. A link γ cuts the elementary surface separating the two quanta and its spin j_γ is the area quantum number of this surface.

diffeomorphisms of Σ. An s-knot state $|s\rangle$ with N nodes represents a quantum excitation of space with N quanta of space adjacent to one another according to the connectivity of Γ (see **Figure 1**).

Notice that the quantum states $|s\rangle$ do not represent quantum excitations living in the physical space: they represent quantum excitations of the physical space. For instance, the state $|0\rangle$ defined by the empty graph does not represent an "empty" physical space, but the absence of any physical space. A generic quantum state of the physical space is represented by a normalizable linear superposition of these discrete quantized spacetimes (*see* Knot Invariants and Quantum Gravity).

In a nongeneral covariant context, the kinematical quantization predictions of quantum theory (such as the quantization of the angular momentum) are obtained from the spectral properties of operators that represent measurements at a given time. In the general covariant Hamiltonian formalism, the corresponding kinematical quantization predictions are given by spectral properties of "partial observables" operators, which in general are not gauge invariant in the sense of Dirac. Area and volume are partial observables of this kind. Their spectra are therefore interpreted as physical predictions of LQG (up to an overall numerical factor, called the Immirzi parameter, which is obtained in certain variants of the theory).

Dynamics

The dynamics of the theory is obtained in terms of a "Hamiltonian constraint" operator C that quantizes the constraint [3]. Different variants of the operator C, and of its Lorentzian version, have been constructed. The operator is defined via a suitable regularization procedure. The description of these constructions exceeds the scope of this article, and we limit ourself here to mentioning the main result and a few general comments.

The main result of the LQG dynamics is that C turns out to be well defined and ultraviolet-finite when restricted to $\mathcal{K}_{\text{diff}}$. Finiteness holds also when standard matter couplings, such as Yang–Mills fields and fermions, are added.

The reason for this finiteness can be understood as a consequence of the discrete nature of space implied by the spectral properties of the geometric operators described above. The limit in which the ultraviolet cutoff, introduced to regulate C, is removed turns out to be trivial on the diffeomorphism-invariant states in $\mathcal{K}_{\text{diff}}$. This is because this limit probes the short-distance regime, but there is no *physical* (gauge-invariant) short distance, in a theory in which geometry turns out to be quantized at the Plank scale. Since the physical states in $\mathcal{K}_{\text{diff}}$ define a physical geometry only at scales larger than the Planck scale $\hbar G c^{-3}$, the "short-distance" modes in the coordinate manifold Σ turn out to be pure gauge. This interplay between quantum field-theoretical and general-relativistic physics is the distinctive character of LQG.

Finally, we sketch the formal structure that dynamics can take in the general covariant Hamiltonian formalism of LQG. The operator C defines a linear operator $P \sim \delta(C)$, usually (improperly) denoted the "projector," which sends states in $\mathcal{K}_{\text{diff}}$ into the kernel of C, formed by the generalized $\mathcal{K}_{\text{diff}}$ vectors that solve the Wheeler–De Witt equation $C\Psi = 0$ (*see* Wheeler–De Witt Theory). Matrix elements of P are interpreted as transition amplitudes between quantum states of space.

Physical predictions for processes that take place in a finite spacetime region $\mathcal{R}$ can be obtained, in principle, as follows. One considers a state $|\Psi\rangle$ representing the result of the measurement of partial observables of the 3D boundary of a spacetime region $\mathcal{R}$. $|\Psi\rangle$ codes the nonrelativistic notions of initial, boundary and final conditions. Then $\langle 0|P|\Psi\rangle$ can be interpreted as a relative probability amplitude associated to this result. A formal expansion of this amplitude in powers of C generates a spinfoam sum (*see* Spin Foams) that can be understood as the "quantum gravity sum over histories" in $\mathcal{R}$.

A systematic technique for computing physical transition amplitudes from the background-independent and nonperturbative formalism of LQG has not yet been developed.

See also: BF Theories; Black Hole Mechanics; Canonical General Relativity; Knot Invariants and Quantum Gravity; Knot Theory and Physics; Quantum Cosmology; Quantum Dynamics in Loop Quantum Gravity; Quantum Geometry and its Applications; Spin Foams; Wheeler–De Witt Theory.

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Lorentzian Geometry

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Introduction

Einstein's (1916) use of differential geometry as an essential tool in his theory of general relativity has long been a motivation for the study of Lorentzian geometry. More recently, the influential monographs of R Penrose (1972) and of S Hawking and G Ellis (1973), the latter still cited by some as the Bible of general relativity, so fascinated differential geometers that Lorentzian geometry took its place alongside of global Riemannian geometry as a worldwide research area.

Let M be a smooth n-dimensional manifold, $n \geq 2$, with a countable basis. A Lorentz metric $g = \langle\, , \rangle$ on M is a symmetric nondegenerate (0, 2) tensor field on M of index $(-, +, \ldots, +)$. The existence of such a tensor field implies that M admits a (non-oriented) line field; hence, some compact manifolds like S^2 do not admit such metrics. A nonzero tangent vector v in TM is then timelike (resp., nonspacelike, null, spacelike) according to whether $g(v, v) < 0$ (resp., ≤ 0, $= 0$, > 0). A Lorentzian manifold (M, g) is a pair consisting of a smooth manifold together with a choice of Lorentz metric. In this article, we use the convention that a spacetime (M, g) is a Lorentzian manifold together with a choice of time orientation, that is, a continuous timelike vector field X on M. Then a tangent vector v based at p may be consistently defined to be future (resp., past) directed if $g(X(p), v) < 0$ (resp., > 0). (Some authors also require that (M, g) be space oriented.) If a Lorentzian manifold happens not to be time orientable, then a 2-fold covering manifold with the induced pullback metric will be time orientable. Also basic are the notations $p \ll q$ (resp., $p \leq q$) if there is a future-directed timelike (resp., nonspacelike) curve from p to q and the corresponding chronological (resp., causal) future of p given by $I^+(p) = \{q \in M;\, p \ll q\}$ and $J^+(p) = \{q \in M;\, p \leq q\}$.

For a Riemannian manifold (N, g_0), the Riemannian distance function

$$d_0 : N \times N \to [0, +\infty) \qquad [1]$$

given by $d_0(p, q) = \inf\{L(c);\, c : [0, 1] \to N$ is a piecewise smooth curve with $c(0) = p$ and $c(1) = q\}$. A fundamental result in global Riemannian geometry is the celebrated Hopf–Rinow theorem.

Hopf–Rinow Theorem *For any Riemannian manifold (N, g_0), the following conditions are equivalent*:

(i) *metric completeness*: (N, d_0) *is a complete metric space*;
(ii) *geodesic completeness*: *for any v in TN, the geodesic $c_v(t)$ in N with initial condition $c_v'(0) = v$ is defined for all values of an affine parameter t*;
(iii) *for some point p in N, the exponential map $\exp_p$ is defined on all of T_pN*;
(iv) *finite compactness*: *every subset K of N that is d_0 bounded has compact closure.*
Moreover, if any one of (i)–(iv) *holds, then (N, g_0) also satisfies*
(v) *minimal geodesic connectedness*: *given any p, q in N, there exists a smooth geodesic segment $c : [0, 1] \to N$ with $c(0) = p, c(1) = q$ and $L(c) = d_0(p, q)$.*

A Riemannian metric for a smooth manifold is then said to be complete if it satisfies any of the above properties (i) through (iv). The Heine–Borel property of basic topology implies (via (iv)) that all Riemannian metrics for a compact manifold are automatically complete and many of the examples studied in basic Riemannian geometry are complete.

Also, if Riem(N) denotes the space of all Riemannian metrics for a smooth manifold N, both geodesic completeness (property (ii) above) and geodesic incompleteness (the failure of property (ii) to hold for all geodesics) are C^0 stable properties on Riem(N), that is, given a complete (resp., incomplete) metric g for N, there exists an open neighborhood U(g) of g in Riem(N) in the Whitney C^0 fine topology such that all Riemannian metrics h in U(g) are complete (resp., incomplete).

For spacetimes (M, g), however, many basic examples furnished by general relativity fail to be geodesically complete and compactness of the underlying smooth manifold M does not imply that the given Lorentz metric g (let alone all Lorentz metrics for M) are complete. Also, the stability of geodesic completeness and incompleteness is more complicated than in the Riemannian case, necessitating concepts like pseudoconvex geodesic systems and disprisonment as studied by Beem and Parker. To summarize, for spacetimes and their associated Lorentzian distance functions, no naive analogs for the Hopf–Rinow theorem are valid. Under additional hypotheses, geodesic completeness may be guaranteed. Marsden noted that a compact spacetime with a homogenous Lorentz metric is geodesically complete. Then Carriere showed that a compact spacetime whose curvature tensor vanishes is geodesically complete. Later Kamishima (assuming constant curvature) and then Romero and Sanchez more generally showed that a compact Lorentzian manifold which admits a timelike Killing field is geodesically complete.

At any point p in a given spacetime, emanating from p are three families of geodesics: timelike, spacelike, and null. It was hoped in the 1960s that possibly continuity arguments could be obtained for different types of geodesic completeness. However, a series of examples showed by the mid-1970s that timelike geodesic completeness, null geodesic completeness, and spacelike geodesic completeness are logically inequivalent. (Here, a given geodesic is said to be complete if it may be extended to be defined for all values of an affine parameter.) Nomizu and Ozeki for Riemannian manifolds showed that any given Riemannian metric g_0 for the smooth manifold N could be made geodesically complete by making a conformal change of metric Ωg_0, where $\Omega : N \to (0, +\infty)$ is a smooth function. Especially in general relativity, such conformal changes are natural because the causal character of tangent vectors and curves (and hence of the basic causality conditions) are preserved. For spacetimes while generally nonspacelike geodesic completeness could not be produced by conformal changes, for some subclasses of spacetimes, such as the strongly causal ones, it was possible with a global conformal change.

For a large class of spacetimes, the warped or multiwarped products (originally inspired by several cosmological models in general relativity and a basic construction from Riemannian geometry), explicit integral criterion involving the warping functions have been given for timelike or null geodesic completeness. Several early examples of this type of result are discussed in Beem *et al.* (1996, pp. 111–112).

Lorentz Distance and the Nonspacelike Cutlocus

For an arbitrary, not necessarily complete, Riemannian manifold (N, g_0), the Riemannian distance function given in eqn [1] is continuous, the metric topology induced by d_0 coincides with the given manifold topology, and $d_0(p, q)$ is finite for all p, q in N. Now, for an arbitrary spacetime (M, g), and p, q in M, if there is no future-directed nonspacelike curve from p to q, set $d(p, q) = 0$; if there is such a curve, let

$$d(p, q) = \sup\{L(c);\ c : [0, 1] \to (M, g) \text{ is a piecewise smooth future-directed nonspacelike curve with } c(0) = p \text{ and } c(1) = q\} \qquad [2]$$

(Unlike the Riemannian case, [2] does not bound $d(p, q)$ from above by $L(c)$ for any selected curve c and hence the Lorentz distance may assume the value $+\infty$.)

This then defines what some authors term the "Lorentzian distance function"

$$d = d(g) : M \times M \to [0, +\infty] \qquad [3]$$

and other authors term "proper time." It is linked to the causal structure of the given spacetime since

$$d(p, q) > 0 \text{ iff } q \text{ is in } I^+(p) \qquad [4]$$

and in place of the triangle inequality for the Riemannian distance function, a reverse triangle inequality holds:

$$\text{if } p \le r \le q, \text{ then } d(p, q) \ge d(p, r) + d(r, q) \qquad [5]$$

Also in the context of eqn [2], a future-directed nonspacelike curve $c : [0, 1] \to M$ from $c(0) = p$ to $c(1) = q$ is defined to be maximal if $L(c) = d(p, q)$. Corresponding to the Riemannian theory, a maximal nonspacelike curve turns out to be a smooth null or timelike geodesic segment.

As mentioned earlier, geodesic completeness is generally not a natural requirement to place on a spacetime. But what emerges from [4] in place of Riemannian completeness is an interplay between the causal properties of the given spacetime and the continuity (and other properties) of the Lorentzian distance function (cf. Beem *et al.* (1996, chapter 4)). At the extreme of totally vicious spacetimes, the Lorentz distance is always $+\infty$. Less drastically, if (M, g) contains a closed timelike curve passing through p, then $d(p, q) = +\infty$ for all q in $J^+(p)$. Also, certain cosmological models contain pairs of points at infinite distance. In general, Lorentzian distance is only lower semicontinuous. Adding upper semicontinuity forces a distinguishing spacetime to be causally continuous. A spacetime is chronological iff $d(p, p) = 0$ for all p in M. At the other extreme from totally vicious spacetimes are globally hyperbolic spacetimes, which share many properties somewhat analogous to complete Riemannian manifolds. The Lorentzian distance function of a globally hyperbolic spacetime is both continuous and finite valued. (Indeed, a strongly causal spacetime is globally hyperbolic iff all Lorentz metrics g' in the conformal class $C(M, g)$ also have finite-valued distance functions $d(g')$.) Second, corresponding to property (v) of the Hopf–Rinow Theorem, these spacetimes all satisfy maximal nonspacelike geodesic connectability: given any p, q in M with $p \leq q$, there exists a future nonspacelike geodesic segment $c : [0, 1] \to M$ with $c(0) = p$, $c(1) = q$ and $L(c) = d(p, q)$.

A basic concept from the calculus of variations is that of a pair of conjugate points along a geodesic segment $c : [0, a] \to (M, g)$. A smooth vector field $J(t)$ along c is said to be a "Jacobi field" if J satisfies the Jacobi differential equation

$$J'' + R(J, c')c' = 0 \qquad [6]$$

where R denotes the curvature tensor. Then $c(t)$, $c(s)$ are said to be conjugate points along c if there exists a nonzero Jacobi field J along c with $J(t) = J(s) = 0$. Much of the basic comparison techniques in global Riemannian geometry involving lengths of geodesics in manifolds satisfying curvature inequalities, such as the "Rauch comparison theorems," the "Toponogov triangle comparison theorem," and volume comparison theorems, were first obtained through Jacobi field techniques (cf. Petersen (1998) for a contemporary account). Later, Riccati equation techniques became more popular (cf. Karcher (1989)). For spacetimes, especially in the globally hyperbolic case, analogous results have been obtained for nonspacelike geodesic segments, with a key breakthrough in 1979 being Harris's version of the "Toponogov triangle comparison theorem" for timelike geodesic triangles in globally hyperbolic spacetimes. The Raychaudhuri equation used earlier in general relativity corresponds for spacetimes to this passage in the Riemannian setting from the Jacobi equation to the Riccati equation. The basic conjugate point theory and the Morse index theory for an arbitrary timelike or null geodesic segment in a general spacetime are reasonably close to the earlier Riemannian theory, if vector fields of the form $J(t) = f(t)\beta'(t)$ are accounted for in the case of a null geodesic segment $\beta : [0, 1] \to (M, g)$. But spacelike geodesics and conjugate points are more problematic, as was first established using symplectic techniques by Helfer in 1994. More recently, progress has been made in applying important ideas of Gromov (1999) for Riemannian manifolds to the spacetime context (cf. Noldus (2004) for an example).

Inspired by fundamental concepts in global Riemannian geometry, Beem and Ehrlich in 1979 introduced the concept of nonspacelike cut point, again most tractable for globally hyperbolic spacetimes. Let $\gamma : [0, a) \to (M, g)$ be a future-inextendible, future-directed nonspacelike geodesic in an arbitrary spacetime. Define

$$t_0 = \sup\{t \in [0, a);\ d(\gamma(0), \gamma(t)) = L(\gamma|_{[0,t]})\} \qquad [7]$$

(If there is a closed timelike curve through $\gamma(0)$, then $d(\gamma(0), \gamma(0)) = +\infty$ and t_0 will not exist. If γ is a nonspacelike geodesic ray and hence $d(\gamma(0), \gamma(t)) = L(\gamma|_{[0,t]})$ for all t, then $t_0 = a$.) However, if $0 < t_0 < a$, then $\gamma(t_0)$ is said to be the future nonspacelike cut point of $p = \gamma(0)$ along γ. For general spacetimes, it may be shown that:

1. for $0 < s < t < t_0$, that $\gamma|_{[s,t]}$ is the unique maximal nonspacelike geodesic in all of (M, g) between $\gamma(s)$ and $\gamma(t)$;
2. $\gamma|_{[0,t]}$ is maximal for all t with $0 \leq t \leq t_0$; and
3. for all t with $t_0 < t < a$, there is a longer nonspacelike curve in (M, g) than $\gamma|_{[0,t]}$ between $\gamma(0)$ and $\gamma(t)$.

A nonspacelike cut point is a subtler concept than a nonspacelike conjugate point since the existence of a cut point is not necessarily captured by the behavior of families of future nonspacelike curves (or geodesics) close to the given geodesic segment γ, the basic viewpoint of the calculus of variations. But since calculus of variations arguments shows that past a nonspacelike conjugate point, longer "neighboring curves" join $\gamma(0)$ to $\gamma(t)$, the future cut point of $p = \gamma(0)$ along γ comes no later than the first

future conjugate point to p along γ in either the timelike or null geodesic case.

In a startling result which contradicted erroneous arguments in all the standard textbooks, Margerin in 1993 gave examples to show that even for compact Riemannian manifolds, the first conjugate locus of a point (i.e., the set of all first conjugate points along all geodesics issuing from a given point) need not be closed, even though elementary arguments correctly show that the cut locus of any point (i.e., the set of all cut points along all geodesics issuing from the given point) is always closed. The timelike first conjugate locus of a point in a spacetime will generally not be closed, but because a nonspacelike geodesic in a globally hyperbolic spacetime must escape from any compact subset in finite affine parameter, the future (or past) first nonspacelike conjugate locus of any point in such a spacetime is a closed subset. In a result analogous to the Riemannian characterization, nonspacelike cut points in globally hyperbolic spacetimes may be characterized as follows: let $q=\gamma(t_0)$ be the future cut point of $p=\gamma(0)$ along the timelike (resp., null) geodesic segment γ from p to q. Then either one of both of the following conditions hold: (1) q is the first future conjugate point to p along γ, or (2) there exist at least two maximal timelike (resp., null) geodesic segments from p to q.

Now given p in an arbitrary spacetime (M, g), the future timelike (resp., null) cut locus of p is defined to be the set of all timelike (resp., null) cut points along all future timelike (resp., null) geodesics issuing from p and the future nonspacelike cut locus of p is defined as the union of the future timelike and null cut loci. Employing alternatives (1) and (2) in the preceeding paragraph, it may be shown for globally hyperbolic spacetimes that the null and nonspacelike cut loci are closed subsets of M.

The null cut locus has a privileged status by virtue of a phenomena not encountered for Riemannian manifolds. Under a conformal change of back-ground spacetime metric, null geodesics remain null pregeodesics (i.e., may be reparametrized to be null geodesics in the deformed Lorentz metric) while such deformations fail to preserve timelike or spacelike geodesics, or to preserve geodesics in the Riemannian case. Even though null conjugate points along a null geodesic will not remain invariant under conformal change of spacetime metric, it is remarkable that elementary arguments involving the spacetime distance function show that global conformal diffeomorphisms do preserve null cut points and hence the null cut locus of any point.

Geodesic Incompleteness and the Lorentzian Splitting Theorem

In global Riemannian geometry, an important concept is that of a geodesic ray. In a complete Riemannian manifold (N, g_0), a unit geodesic $c:[0,+\infty) \to (N, g_0)$ is said to be a (geodesic) ray if $d_0(c(0), c(t))=t$ for all $t \geq 0$. By the triangle inequality, $c(t)$ is minimal between every pair of its points. By making a limit construction, it may be shown that for each p in N, there exists a geodesic ray $c(t)$ with $c(0)=p$. An allied concept is that of a (geodesic) line $c:\mathbb{R} \to (N, g_0)$; here $d_0(c(t), c(s))=|t-s|$ for all t, s is required, that is, c is minimal between every pair of its points. The existence of a line is much stronger than the existence of a ray. If (N, g_0) has positive Ricci curvature everywhere, then (N, g_0) contains no lines despite the fact that it contains a ray issuing from each point. A helpful tool in this setting is the compactness of sets of tangent vectors of the form

$$\{w \in T_pN;\ g_0(w, w) = 1\} \qquad [8]$$

for any p in N; hence, any infinite sequence of tangent vectors based at p automatically has a convergent subsequence.

For spacetimes, geodesic completeness cannot generally be assumed. Yet a future nonspacelike geodesic ray $\gamma : [0, b) \to (M, g)$ may be defined to be a future-directed, future-inextendible nonspacelike geodesic with $d(\gamma(0), \gamma(t))=L(\gamma|_{[0,t]})$ for all t in $[0, b)$. The reverse triangle inequality implies that γ is maximal between any pair of its points. Similarly, a nonspacelike geodesic line $\gamma : (a, b) \to (M, g)$ is a past- and future-inextendible nonspacelike geodesic with $d(\gamma(t), \gamma(s))=L(\gamma|_{[t,s]})$ for all s, t. Hence, γ is maximal between any pair of its points. If nonspacelike geodesic completeness is assumed, $a=-\infty$ and $b=+\infty$ above. Constructions here are more delicate than in the Riemannian case because the sets

$$\{v \in T_pM;\ g(v, v) = -1\} \qquad [9]$$

of unit timelike tangent vectors, while closed in the tangent space, are noncompact. Despite this technicality, using the limit curve machinery of general relativity in place of the compactness in [8], it has been shown that a strongly causal spacetime admits a past and future nonspacelike geodesic ray issuing from every point (cf. Beem *et al.* (1996, chapter 8)). (If the spacetime is not nonspacelike geodesically complete, these rays will not necessarily be past or future complete.) As in the Riemannian case, the existence of a complete line is a stronger geometric condition. For that reason, in 1977 Beem and Ehrlich introduced the concept of a spacetime causally disconnected by a compact set K and

showed that a strongly causal spacetime which is causally disconnected by a compact set contains a nonspacelike geodesic line which intersects the compact set. (Again, unless the spacetime is nonspacelike geodesically complete, this line need not be future or past complete.)

A pattern common to many results in global Riemannian geometry especially since the 1950s is the following: the existence of a complete Riemannian metric on a smooth manifold which also satisfies a global curvature inequality implies a topological or geometric conclusion. A celebrated early example from the 1950s and 1960s, obtained by separate results of Rauch, Berger, and Klingenberg, is the topological sphere theorem.

Topological Sphere Theorem *Suppose* (N, g_0) *is a complete, simply connected Riemannian n-manifold whose sectional curvatures satisfy* $1/4 < K \leq 1$. *Then N is homeomorphic to* S^n.

By contrast, for spacetimes, the assumption of geodesic completeness is generally unwarranted. Here is an example of one of the celebrated singularity theorems of general relativity, published in 1970 as originally stated:

Hawking–Penrose Singularity Theorem *No spacetime* (M, g) *of dimension* $n \geq 3$ *can satisfy all of the following three requirements together*:

(i) (M, g) *contains no closed timelike curves*;
(ii) *Every inextendible nonspacelike geodesic in* (M, g) *contains a pair of conjugate points*; *and*
(iii) *There exists a future- or past-trapped set S in* (M, g).

This theorem may be reinterpreted more akin to the Riemannian pattern above as follows: suppose (M, g) is a chronological spacetime of dimensions $n \geq 3$ which satisfies the timelike convergence condition ($\mathrm{Ric}(v, v) \geq 0$ for all timelike tangent vectors) and the generic condition (every inextendible nonspacelike geodesic contains a point which has some appropriate nonzero sectional curvature). If (M, g) contains a future- or past-trapped set, then (M, g) is nonspacelike geodesically incomplete. Hence, this result models the pattern: global curvature inequalities (reflecting the physical assumptions that gravity is assumed to be attractive and every inextendible nonspacelike geodesic experiences tidal acceleration) and a further physical or geometric assumption (the first and third conditions) implies the existence of an incomplete timelike or null geodesic.

An influential concept in global Riemannian geometry formulated during the 1960s and 1970s is that of curvature rigidity, which first became widely known through the introduction to the text Cheeger and Ebin (1975). The above statement of the "sphere theorem" contains one hypothesis that the sectional curvature is strictly greater than 1/4. In curvature rigidity, the hypothesis of strict inequality is relaxed to include the possibility of equality as well, and then one tries to show that either the old conclusion is still valid, or if it fails, it fails in an isometric (hence "rigid") manner. Thus in the example of the sphere theorem, if the sectional curvature is now allowed to satisfy $1/4 \leq K \leq 1$, then either the given Riemannian manifold remains homeomorphic to the n-sphere, or if not, it is isometric to a Riemannian symmetric space of rank 1.

Already in an article in 1970, Geroch had expressed the opinion that most spacetimes should be nonspacelike geodesically incomplete and also that a spacetime should fail to be nonspacelike geodesically incomplete only under special circumstances. Apparently by the early 1980s, S T Yau had formulated the idea that timelike geodesic incompleteness of spacetimes ought to display a curvature rigidity. In the paragraph following the statement of the Hawking–Penrose singularity theorem, there are two curvature conditions mentioned – the timelike convergence condition and the generic condition. Now the timelike convergence condition already allows for the case of equality (i.e., zero timelike Ricci curvature) in its formulation; hence, curvature rigidity here would imply dropping the generic condition that each inextendible nonspacelike geodesic contains a point of nonzero sectional curvatures as a hypothesis. This notion seems first to have been published by Yau's Ph.D. student R Bartnik in 1988 as follows:

Conjecture *Let* (M, g) *be a spacetime of dimension* ≥ 3 *which*

(i) *contains a compact Cauchy surface and*
(ii) *satisfies the timelike convergence condition* $Ric(v, v) \geq 0$ *for all timelike v*.

Then either (M, g) *is timelike geodesically incomplete, or* (M, g) *splits isometrically as a product* $(\mathbb{R} \times V, -\mathrm{d}t^2 + h)$ *where* (H, h) *is a compact Riemannian manifold.*

This conjecture has been proven in many cases with the following proof scheme. From the physical or geometric assumptions made, produce an inextendible nonspacelike geodesic line. Further, prove that the line happens to be timelike rather than null. Then if the spacetime were timelike geodesically complete, it would contain a complete

timelike line. But then the desired splitting may be obtained using the Lorentzian splitting theorem.

Lorentzian Splitting Theorem *Let (M, g) be a spacetime of dimension ≥ 3 which satisfies each of the following conditions:*

(i) *(M, g) is either globally hyperbolic or timelike geodesically complete;*
(ii) *(M, g) satisfies the timelike convergence condition; and*
(iii) *(M, g) contains a complete timelike line.*

Then (M, g) splits isometrically as a product $(\mathbb{R} \times V, -dt^2 + h)$ where (H, h) is a complete Riemannian manifold.

This result, which corresponds to obtaining the spacetime analog of a celebrated splitting theorem of Cheeger and Gromoll for lines in complete Riemannian manifolds of non-negative Ricci curvature, published in 1971, was posed as a problem by S T Yau in a problem list stemming from the conference Special Year in Differential Geometry held at the Institute for Advanced Study in Princeton during the 1979–80 academic year. Early progress was made using maximal hypersurface methods by Gerhardt in 1983, Bartnik in 1984, and Galloway in 1984. Then in 1985, Beem, Ehrlich, Markvorsen, and Galloway introduced the methodology of employing the Busemann function of the complete timelike line, motivated by techniques from Riemannian geometry, and succeeded in obtaining a splitting under the hypothesis of global hyperbolicity and everywhere nonpositive timelike sectional curvatures. In separate publications, Eschenburg and Galloway extended the result to the desired curvature hypothesis of nonnegative timelike Ricci curvatures. Finally, Newman in 1990 achieved the originally desired goal of obtaining the splitting under the assumption of timelike geodesic completeness, rather than global hyperbolicity. This is a more delicate setting, since timelike geodesic completeness does not imply maximal nonspacelike geodesic connectability, a fairly basic geometric tool in many standard constructions. But the idea emerged with Newman's solution that the existence of a timelike geodesic line or segment in a nonglobally hyperbolic spacetime implies an adequate level of control in a tubular neighborhood of the given line to enable the proof to work. Galloway and Horta in 1996 published a much simplified working out of these concepts. A fuller exposition of these developments may be found in Beem *et al.* (1996, chapter 14). In addition, in 2000, Galloway published a version of the splitting theorem for a null maximal geodesic line.

Two-Dimensional Spacetimes

Two-dimensional spacetimes, sometimes termed Lorentz surfaces, are especially tractable because given (M, g) with $\dim M = 2$, then $(M, -g)$ is also a spacetime. Hence, it may be shown that any Lorentzian 2-manifold (M, g) homeomorphic to $\mathbb{R}^2$ may be made geodesically complete (not just nonspacelike geodesically complete) by a conformal change of metric. Also, any simply connected two-dimensional Lorentzian manifold is strongly causal. In Weinstein (1996), an extensive study is made of Lorentz surfaces generally and particularly, of a conformal boundary for such surfaces first given by Kulkarni in 1985.

One of the prettiest classical results linking the geometry and topology of a Riemannian surface is the Gauss–Bonnet theorem. Let (N, g_0) be a Riemannian manifold of dimension 2 and let P be a polygonal subregion with piecewise smooth bounding curves c_i, $1 \leq i \leq k$. Let K denote the Gauss curvature of (N, g_0) and κ the geodesic curvature of the smooth curves c_i (which vanishes if c_i happens to be a geodesic). If α_i denote the corresponding interior angles between the successive boundary curves c_i and c_{i+1}, then the Gauss–Bonnet formula over P is

$$\int_P\!\!\int K\, dA + \int_{\partial P} \kappa\, ds + \sum_i (\pi - \alpha_i) = 2\pi \qquad [10]$$

By considering a triangulation of N itself and summing up the corresponding terms in [10], it follows for a compact oriented Riemannian manifold (N, g_0) of dimension 2 that

$$\int_N\!\!\int K\, dA = 2\pi\chi_{(N)} \qquad [11]$$

where $\chi_{(N)}$ denotes the Euler characteristic. Also lurking in the background here is a formula for computing the angle between unit tangent vectors v, w as

$$\cos\theta = g_0(v, w) \qquad [12]$$

In the spacetime setting, different versions of a Gauss–Bonnet formula for subregions of a two-dimensional spacetime (M, g) corresponding to [10] have been given in 1974 by Helzer and in 1984 by Birman and Nomizu. First, the angle computation is a bit trickier for spacetimes than in the Riemannian case; eqn [12] has to be replaced by techniques which use the hyperbolic functions $\cosh u$ and $\sinh u$ to define the angle u (sometimes called the "hyperbolic angle") between two unit vectors and

then to allow for null vectors. Birman and Nomizu obtained an analog of [10] assuming that the boundary curves for P are successive smooth unit timelike curves:

$$\int_{\partial P} \kappa \, ds - \int_P \int K \, dA + \sum_i \theta_i = 0$$

Helzer in his formulation allows the different boundary curves to be either unit timelike, unit spacelike or null separately. Since the only compact, orientable smooth surface which admits a spacetime metric is the 2-torus, which has zero Euler characteristic, the Riemannian formula [11] above translates into the uniform constraint on the Gauss curvature of the spacetime:

$$\int_M \int K \, dA = 0$$

See also: General Relativity: Overview; Geometric Analysis and General Relativity; Pseudo-Riemannian Nilpotent Lie Groups; Spacetime Topology, Causal Structure and Singularities.

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Lyapunov Exponents and Strange Attractors

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Lyapunov Exponents

The Lyapunov exponents of a sequence $\{A^n, n \geq 1\}$ of square matrices of dimension $d \geq 1$ are the values of

$$\lambda(v) = \limsup_{n \to \infty} \frac{1}{n} \log \|A^n \cdot v\| \qquad [1]$$

over all nonzero vectors $v \in \mathbb{R}^d$. For completeness, set $\lambda(0) = -\infty$. It is easy to see that $\lambda(cv) = \lambda(v)$ and $\lambda(v + v') \leq \max\{\lambda(v), \lambda(v')\}$ for any nonzero scalar c and any vectors v, v'. It follows that, given any constant a, the set of vectors satisfying $\lambda(v) \leq a$ is a vector subspace. Consequently, there are at most d Lyapunov exponents, henceforth denoted by $\lambda_1 < \cdots < \lambda_{k-1} < \lambda_k$, and there exists a filtration $F^1 < \cdots < F^{k-1} < F^k = \mathbb{R}^d$ into vector subspaces, such that

$$\lambda(v) = \lambda_i \quad \text{for all } v \in F_i \backslash F_{i-1}$$

and every $i = 1, \ldots, k$ (write $F_0 = \{0\}$). In particular, the largest exponent is

$$\lambda_k = \limsup_{n \to \infty} \frac{1}{n} \log \|A^n\| \qquad [2]$$

One calls $\dim F_i - \dim F_{i-1}$ the multiplicity of each Lyapunov exponent λ_i.

There are corresponding notions for continuous families of matrices $A^t, t \in (0, \infty)$, taking the limit as t goes to ∞ in the relations [1] and [2]. The theories for the two types of families, discrete and continuous, are analogous and so at each point in what follows we refer to either one or the other.

Lyapunov Stability

Consider the linear differential equation

$$\dot{v}(t) = B(t) \cdot v(t) \qquad [3]$$

where $B(t)$ is a bounded function with values in the space of $d \times d$ matrices, defined for all $t \in \mathbb{R}$. The theory of differential equations ensures that there exists a fundamental matrix $A^t, t \in \mathbb{R}$, such that

$$v(t) = A^t \cdot v_0$$

is the unique solution of [3] with initial condition $v(0) = v_0$.

If the Lyapunov exponents of the family $A^t, t > 0$, are all negative then the trivial solution $v(t) \equiv 0$ is asymptotically stable, and even exponentially stable. The stability theorem of Lyapunov asserts that, under an additional regularity condition, stability is still valid for nonlinear perturbations

$$w(t) = B(t) \cdot w + F(t, w) \qquad [4]$$

with $\|F(t,w)\| \le \text{const.}\|w\|^{1+c}, c > 0$. That is, the trivial solution $w(t) \equiv 0$ is still exponentially asymptotically stable.

The regularity condition means, essentially, that the limit in [1] does exist, even if one replaces vectors v by elements $v_1 \wedge \cdots \wedge v_l$ of any lth exterior power of $\mathbb{R}^d, 1 \le l \le d$. By definition, the norm of an l-vector $v_1 \wedge \cdots \wedge v_l$ is the volume of the parallelepiped determined by the vectors $v_1, \ldots, v_k$. This condition is usually tricky to check in specific situations. However, the multiplicative ergodic theorem of VI Oseledets asserts that, for very general matrix-valued stationary random processes, regularity is an almost sure property. This result sets the foundation for the modern theory of Lyapunov exponents. We are going to discuss the precise statement of the theorem in the slightly broader setting of linear cocycles, or vector bundle morphisms.

Linear Cocycles

Let μ be a probability measure on some space M and $f: M \to M$ be a measurable transformation that preserves μ. Let $\pi: \mathcal{E} \to M$ be a finite-dimensional vector bundle, endowed with a Riemannian metric $\|\cdot\|_x$ on each fiber $\mathcal{E}_x = \pi^{-1}(x)$. Let $\mathcal{A}: \mathcal{E} \to \mathcal{E}$ be a linear cocycle over f. What we mean by this is that

$$\pi \circ \mathcal{A} = f \circ \pi$$

and the action $A(x): \mathcal{E}_x \to \mathcal{E}_{f(x)}$ of $\mathcal{A}$ on each fiber is a linear isomorphism. Notice that the action of the nth iterate $\mathcal{A}^n$ is given by

$$A^n(x) = A(f^{n-1}(x)) \cdots A(f(x)) \cdot A(x)$$

for every $n \ge 1$.

Assume the function $\log^+ \|A(x)\|_x$ is μ-integrable:

$$\log^+ \|A(x)\|_x \in L^1(\mu) \qquad [5]$$

(we write $\log^+ \phi = \log \max\{\phi, 1\}$, for any $\phi > 0$). It is clear that the sequence of functions $a_n(x) = \log \|A^n(x)\|_x$ satisfies

$$a_{m+n}(x) \le a_m(x) + a_n(f^m(x))$$

for every m, n, and x. It follows from J Kingman's subadditive ergodic theorem that the limit

$$\lim_{n \to \infty} \frac{1}{n} a_n(x)$$

exists for μ-almost all x. In view of [2], this means that the largest Lyapunov exponent $\lambda_k(x)$ of the sequence $A^n(x), n \ge 1$ is a limit, and not just a lim sup, at almost every point.

Multiplicative Ergodic Theorem

The Oseledets theorem states that the same holds for all Lyapunov exponents. Namely, for μ-almost every $x \in M$ there exists $k = k(x) \in \{1, \ldots, d\}$, a filtration

$$F_x^1 < \cdots < F_x^{k-1} < F_x^k = \mathcal{E}_x$$

and numbers $\lambda_1(x) < \cdots < \lambda_k(x)$ such that

$$\lim_{n \to \infty} \frac{1}{n} \log \|A^n(x)\|_x = \lambda_i(x) \qquad [6]$$

for all $v \in F_x^i \setminus F_x^{i-1}$ and $i \in \{1, \ldots, k\}$.

The Lyapunov exponents $\lambda_i(x)$, and their number $k(x)$, are measurable functions of x and they are constant on orbits of the transformation f. In particular, if the measure μ is ergodic then k and the λ_i are constant on a full μ-measure set of points. The subspaces F_x^i also depend measurably on the point x and are invariant under the linear cocycle:

$$A(x) \cdot F_x^i = F_{f(x)}^i$$

It is in the nature of things that, usually, these objects are not defined everywhere and they depend discontinuously on the base point x.

When the transformation f is invertible, one obtains a stronger conclusion, by applying the previous kind of result also to the inverse of the cocycle. Namely, assuming that $\log^+ \|A^{-1}\|$ is also in $L^1(\mu)$, one gets that there exists a decomposition

$$\mathcal{E}_x = E_x^1 \oplus \cdots \oplus E_x^k$$

defined at almost every point and such that $A(x) \cdot E^i_x = E^i_{f(x)}$ and

$$\lim_{n\to\pm\infty} \frac{1}{n} \log \|A^n(x)\|_x = \lambda_i(x) \qquad [7]$$

for all $v \in E^i_x$ different from zero and all $i \in \{1, \ldots, k\}$. These Oseledets subspaces E^i_x are related to the subspaces F^i_x through

$$F^j_x = \bigoplus_{i=1}^{j} E^i_x$$

Hence, $\dim E^i_x = \dim F^i_x - \dim F^{i-1}_x$ is the multiplicity of the Lyapunov exponent $\lambda_i(x)$.

The angles between any two Oseledets subspaces decay subexponentially along orbits of f:

$$\lim_{n\to\pm\infty} \frac{1}{n} \log \text{angle}\left(E^i_{f^n(x)}, E^j_{f^n(x)}\right) = 0$$

for every $i \neq j$ and almost every point. These facts imply the regularity condition mentioned previously and, in particular,

$$\lim_{n\to\pm\infty} \frac{1}{n} \log |\det A^n(x)| = \sum_{i=1}^{k} \lambda_i(x) \dim E^i_x \qquad [8]$$

Consequently, for cocycles with values in $SL(d, \mathbb{R})$, the sum of all Lyapunov exponents, counted with multiplicity, is identically zero.

As we are dealing with almost certain properties, we may generally restrict the vector bundle to some full measure subset over which it is trivial. Then each fiber $\mathcal{E}_x$ is identified with the space $\mathbb{R}^d$, and we may think of $A(x)$ as a $d \times d$ matrix. Then $A_n(x) = A(f^n(x))$ is a stationary random process relative to (f, μ). Thus, in this context it is no serious restriction to view a linear cocycle as a stationary random process with values in the linear group $GL(d, \mathbb{R})$ of invertible $d \times d$ matrices.

Furthermore, given any such random process $A_n, n \geq 0$, one may consider its normalization $B_n = A_n / |\det A_n|$. The Lyapunov exponents of the two random processes $A_n, n \geq 0$, and $B_n, n \geq 0$, differ by the time average

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} \log |\det A_j(x)|$$

of the determinant. The Birkhoff ergodic theorem ensures that the time average is well defined almost everywhere, as long as the function $\log|\det A|$ is in $L^1(\mu)$; this is the case, for instance, if both $\log^+ \|A^{\pm 1}\|$ are integrable. This relates the general case to random processes with values in the special linear group $SL(d, \mathbb{R})$ of $d \times d$ matrices with determinant ± 1.

The Oseledets theorem was extended by D Ruelle to certain linear cocycles in infinite dimensions. He assumes that the $A(x)$ are compact operators on a Hilbert space H and $\log^+ \|A\|$ is in $L^1(\mu)$. The conclusion is the same as in finite dimensions, except that the filtration

$$\cdots < F^i_x < \cdots < F^1_x = H$$

may involve infinitely many subspaces, and the Lyapunov exponents may be $-\infty$. There is also a version for cocycles over invertible transformations, where one assumes each $A(x)$ to be invertible and the sum of a unitary operator with a compact operator, such that both $\log\|A^{\pm}\|$ are integrable. The conclusion is that there exists an Oseledets decomposition $H = E^1_x \oplus \cdots \oplus E^i_x \oplus \cdots$ at almost every point, with finitely or countably many factors.

Random Matrices

Relation [8] implies that, for $SL(d, \mathbb{R})$ cocycles, if there is only one Lyapunov exponent (with full multiplicity) then it must be zero. When this happens, the theory contains no information on the behavior of the iterates $A^n(x) \cdot v$, apart from the fact that there is no exponential growth nor decay of their norms. Thus, the question naturally arises under which conditions is there more than one Lyapunov exponent or, equivalently, under which conditions is the largest Lyapunov exponent strictly positive.

This problem was first addressed by H Furstenberg for products of independent random variables, corresponding to the following class of linear cocycles. Let ν be a probability measure on the group $G = GL(d, \mathbb{R})$. Consider $M = G^{\mathbb{N}}$ and $\mu = \nu^{\mathbb{N}}$ (or $M = G^{\mathbb{Z}}$ and $\mu = \nu^{\mathbb{Z}}$), and let $f: M \to M$ be the shift map

$$f\left((\alpha_j)_j\right) = (\alpha_{j+1})_j$$

It is clear that μ is invariant and also ergodic for the transformation f. Consider the cocycle $\mathcal{A}: \mathcal{E} \to \mathcal{E}$ defined by $\mathcal{E} = M \times \mathbb{R}^d$ and

$$A\left((\alpha_j)_j\right) \cdot v = \alpha_0 \cdot v$$

Clearly,

$$A^n\left((\alpha_j)_j\right) \cdot v = \alpha_{n-1} \cdots \alpha_1 \alpha_0 \cdot v$$

Corresponding to the hypothesis of the multiplicative ergodic theorem, assume that $\log^+ \|\alpha\|$ (and $\log^+ \|\alpha^{-1}\|$) are ν-integrable functions of the matrix α.

Furstenberg's theorem states that if the closed group $G(\nu)$ generated by the support of ν is

noncompact and strongly irreducible in $\mathbb{R}^d$ then the largest Lyapunov exponent of the cocycle $\mathcal{A}$ is strictly positive. Strong irreducibility means that there exists no finite union of subspaces of $\mathbb{R}^d$ that is invariant under all elements of the group. Improvements, extensions, and alternative proofs have been obtained by several authors since then.

Especially, Y Guivarc'h and A Raugi provided conditions under which there are exactly d distinct Lyapunov exponents or, in other words, the multiplicity of every Lyapunov exponent is equal to 1. A matrix semigroup has the contraction property if there exists a sequence of elements h_n and a probability measure on the projective space of $\mathbb{R}^d$ that gives zero weight to any projective subspace, such that the images $(h_n)_* m$ of m under the h_n converge to a Dirac mass in the projective space. They proved that if the closed semigroup $H(\nu)$ generated by the support of the probability ν is strongly irreducible and has the contraction property then the largest Lyapunov exponent has multiplicity 1. Applying this to the exterior powers of the cocycle, one obtains sufficient conditions for simplicity of the other Lyapunov exponents as well.

This statement has been improved by I Ya Gol'dsheid and G A Margulis, who formulated the hypotheses in terms of the algebraic closure $\tilde{G}(\nu)$ of the semigroup $H(\nu)$. They assumed that $\tilde{G}(\nu)$ has the contraction property and the connected component of the identity inside $\tilde{G}(\nu)$ is irreducible in $\mathbb{R}^d$, meaning that its elements do not have any common invariant subspace. Then the largest Lyapunov exponent is simple.

Schrödinger Cocycles

The one-dimensional discrete Schrödinger equation is the second-order difference equation

$$-(u_{n+1} + u_{n-1}) + V_n u_n = E u_n \qquad [9]$$

derived from the stationary Schrödinger equation in dimension 1 by space discretization. Here the energy E is a constant and $V_n = V(f^n(\theta))$, where the potential $V(\cdot)$ is a bounded scalar function and $f: M \to M$ is a transformation preserving some probability measure μ on M. In what follows, we take μ to be ergodic. Equation [9] may be rewritten as a first-order relation,

$$\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} V_n - E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix}$$

Hence, it may also be interpreted as a linear cocycle $\mathcal{A}$ over f, where the vector bundle is $\mathcal{E} = M \times \mathbb{R}^2$ and

$$A(\theta) = \begin{pmatrix} V(\theta) - E & -1 \\ 1 & 0 \end{pmatrix} \qquad [10]$$

takes values in $SL(\mathbb{R}, 2)$. By ergodicity, the Lyapunov exponents are essentially independent of the base point θ. Let $\lambda(E)$ denote the largest exponent: by the relation [8], the other one is $-\lambda(E)$.

The Lyapunov exponent $\lambda(E)$ is related to the spectral theory of the linear operators $\mathcal{L}_\theta$,

$$(\mathcal{L}_\theta u)_n = -(u_{n+1} + u_{n-1}) + V_n u_n$$

on the space $\ell^2(\mathbb{Z})$ of complex square-integrable sequences u_n, $n \in \mathbb{Z}$. These are bounded Hermitian operators and so the spectra are compact subsets of $\mathbb{R}$. Using the assumption that μ is ergodic, one can prove that the spectrum $\mathrm{spec}(\mathcal{L}_\theta)$ is constant almost everywhere. If the transformation f is minimal, the spectrum is even independent of the point θ. Moreover, for all energies,

$$\lambda(E) \geq \text{const. } \mathrm{dist}(E, \mathrm{spec}(\mathcal{L}_\theta))$$

In particular, $\lambda(E)$ is always positive on the complement of the spectrum.

A fundamental problem (Anderson localization) is to decide when the spectrum is pure-point. This is reasonably well understood for a few classes of base dynamics only, for example, the very chaotic systems such as Bernoulli and Markov processes (random potentials) or uniformly hyperbolic maps and flows, or the irrational rotations on the d-dimensional torus (quasiperiodic potentials). In the latter case, the results are more complete when there is only one frequency ($d = 1$). It was shown by K Ishii and by L Pastur that if $\lambda(E)$ is positive for almost all values of E in some Borel set then the absolutely continuous part of the spectrum is essentially disjoint from that set. The converse is also true (due to S Kotani). Thus, checking that $\lambda(E)$ is positive is an important step towards proving localization.

A very general criterion for positivity of the Lyapunov exponent was obtained by Kotani. Namely, he proved that if the potential is not deterministic then $\lambda(E)$ is positive for almost all E. In particular, for nondeterministic potentials the absolutely continuous spectrum is empty, almost surely. In simple terms, the hypothesis means that from the values of the potential for negative n one cannot determine the values for positive n. More formally, one calls the potential deterministic if every $V_n, n \geq 0$ is almost everywhere a measurable function of $\{V_n : n \leq 0\}$. For instance, quasiperiodic potentials are deterministic, whereas Bernoulli potentials are not.

Subharmonicity Method

Let $\mathbb{D}^m$ be the set of complex vectors $(z_1, \ldots, x_m) \in \mathbb{C}^m$ such that $|z_j| \leq 1$ for all j and let $\mathbb{T}^m$ be the subset defined by $|z_j| = 1$ for all j. Let $f: \mathbb{T}^m \to \mathbb{T}^m$ and $A: \mathbb{T}^m \to \mathrm{SL}(d, \mathbb{R})$ be continuous maps that admit holomorphic extensions to the interior of $\mathbb{D}^m$ with $f(0) = 0$. Assume that f preserves the natural (Haar) measure μ on $\mathbb{T}^m$. Let

$$\lambda(A, \mu) = \int_{\mathbb{T}^m} \lambda(z) \mathrm{d}\mu$$

where $\lambda(z)$ denotes the largest Lyapunov exponent for the cocycle defined by A over f. It also follows from the subadditive ergodic theorem that

$$\lambda(A, \mu) = \lim \frac{1}{n} \int_{\mathbb{T}^m} \log \|A^n(z)\| \mathrm{d}\mu$$

M Herman observed that, since the function $\log \|A^n(z)\|$ is plurisubharmonic on $\mathbb{D}^m$, one may use the maximum principle to conclude that

$$\frac{1}{n} \int_{\mathbb{T}^m} \log \|A^n(z)\| \mathrm{d}\mu \geq \frac{1}{n} \log \|A^n(0)\|$$

Then, taking the limit when $n \to \infty$ one obtains that

$$\lambda(A, \mu) \geq \rho(A) \qquad [11]$$

where $\rho(A)$ denotes the spectral radius of the matrix $A(0)$. Starting from this observation, he developed a very effective method for bounding Lyapunov exponents from below, that received several applications and extensions, in particular, to the theory of Schrödinger cocycles with quasiperiodic potentials.

The best-known application is the following bound for integrated Lyapunov exponents of two-dimensional cocycles. Let $f: M \to M$ be a continuous transformation on a compact metric space, preserving some probability measure μ, and $A: M \to \mathrm{SL}(2, \mathbb{R})$ be a continuous map. For each fixed θ, let AR_θ be the cocycle obtained by multiplying $A(x)$, at every point x, by the rotation of angle θ. Herman proved that

$$\frac{1}{2\pi} \int \lambda(AR_\theta, \mu) \mathrm{d}\theta \geq \int_M N(x)\, \mathrm{d}\mu$$

(A Avila and J Bochi later showed that the equality holds) where

$$N(x) = \log \frac{\|A(x)\| + \|A(x)^{-1}\|}{2}$$

Apart from the exceptional case when A acts by rotation at every point in the support of μ, the right-hand side of the inequality is positive, and so the Lyapunov exponent of the cocycle AR_θ is positive for many values of θ.

Nonuniform Hyperbolicity

The prototypical example of a linear cocycle is the derivative of a smooth transformation on a manifold. More precisely, let M be a finite-dimensional manifold and $f: M \to M$ be a diffeomorphism, that is, a bijective smooth map whose derivative $Df(x)$ depends continuously on x and is an isomorphism at every point. Let $\mathcal{E} = TM$ be the tangent bundle to the manifold and $\mathcal{A} = Df$ be the derivative. If M is compact or, more generally, if the norms of both Df and its inverse are bounded, then the hypothesis in Oseledets theorem is automatically satisfied for any f-invariant probability μ. Lyapunov exponents yield deep geometric information on the dynamics of the diffeomorphism, especially when they do not vanish. For most results that we mention in the sequel, one needs the derivative Df to be Hölder continuous:

$$\|Df(x) - Df(y)\| \leq \mathrm{const.}\, d(x, y)^c$$

Let E_x^s be the sum of the Oseledets subspaces corresponding to negative Lyapunov exponents. Pesin's stable manifold theorem states that there exists a family of embedded disks $W_{\mathrm{loc}}^s(x)$ tangent to E_x^s at almost every point and such that the orbit of every $y \in W_{\mathrm{loc}}^s(x)$ is exponentially asymptotic to the orbit of x. This lamination $\{W^s(x)\}$ is invariant, in the sense that

$$f(W^s(x)) \subset W^s(f(x))$$

and has an "absolute continuity" property. There are analogous results for the sum E_x^u of the Oseledets subspaces corresponding to positive Lyapunov exponents.

The entropy of a partition $\mathcal{P}$ of M is defined by

$$h_\mu(f, \mathcal{P}) = \lim_{n \to \infty} \frac{1}{n} H_\mu(\mathcal{P}^n)$$

where $\mathcal{P}^n$ is the partition into sets of the form $P = P_0 \cap f^{-1}(P_1) \cap \cdots \cap f^{-n}(P_n)$ with $P_j \in \mathcal{P}$ and

$$H_\mu(\mathcal{P}^n) = \sum_{P \in \mathcal{P}^n} -\mu(P) \log \mu(P)$$

The Kolmogorov–Sinai entropy $h_\mu(f)$ of the system is the supremum of $h_\mu(f, \mathcal{P})$ over all partitions $\mathcal{P}$ with finite entropy. The Ruelle–Margulis inequality says that $h_\mu(f)$ is bounded above by the average sum of the positive Lyapunov exponents. A major result of the theory, Pesin's entropy formula, asserts that if the invariant measure μ is smooth (e.g., a volume element) then the two invariants coincide:

$$h_\mu(f) = \int \left(\sum_{j=1}^{k} \lambda_j^+ \right) \mathrm{d}\mu$$

A complete characterization of the invariant measures for which the entropy formula is true was given by F Ledrappier and L S Young.

The invariant measure μ is called hyperbolic if all Lyapunov exponents are nonzero at almost every point. Hyperbolic measures are exact dimensional: the pointwise dimension

$$d(x) = \lim_{r \to 0} \frac{\log \mu(B_r(x))}{\log r}$$

exists at almost every point, where $B_r(x)$ is the neighborhood of radius r around x. This fact was proved by L Barreira, Ya Pesin, and J Schmeling. Note that it means that the measure $\mu(B_r(x))$ of neighborhoods scales as $r^{d(x)}$ when the radius r is small.

Another remarkable feature of hyperbolic measures, proved by A Katok, is that periodic motions are dense in their supports. More than that, assuming the measure is nonatomic, there exist Smale horseshoes H_n with topological entropy arbitrarily close to the entropy $h_\mu(f)$ of the system. In this context, the topological entropy $h(f, H_n)$ may be defined as the exponential rate of growth,

$$\lim_{k \to \infty} \frac{1}{k} \log \#\{x \in H_n\colon f^k(x) = x\}$$

of the number of periodic points on H_n.

Generic Systems

Given any area-preserving diffeomorphism on any surface M, one may find another whose first derivative is arbitrarily close to the initial one and which has Lyapunov exponents identically zero at almost every point, or else is globally uniformly hyperbolic (Anosov). This surprising fact was discovered by R Mañé, and a complete proof was given by J Bochi. Uniform hyperbolicity means that the tangent bundle admits a Df-invariant splitting

$$TM = E^{\mathrm{s}} \oplus E^{\mathrm{u}}$$

such that the line bundle E^{s} is uniformly contracted and E^{u} is uniformly expanded by the derivative. It is well known that Anosov diffeomorphisms can only occur if the surface is the torus $\mathbb{T}^2$.

In fact, the theorem of Mañé–Bochi is stronger: for a residual subset (a countable intersection of open dense sets) of all once-differentiable area-preserving diffeomorphisms on any surface, either the Lyapunov exponents vanish almost everywhere or the diffeomorphism is Anosov. This shows that zero Lyapunov exponents are actually quite common for surface diffeomorphisms that are only once-differentiable. Moreover, this theorem has been extended to diffeomorphisms on manifolds with arbitrary dimension, in a suitable formulation, by J Bochi and M Viana.

However, this phenomenon should be specific to systems with low differentiability. Indeed, already for Hölder-continuous linear cocycles over chaotic transformations it is known that vanishing Lyapunov exponents can only occur with infinite codimension. That is, unless the cocycle satisfies an infinite number of independent constraints, there exists some positive exponent. By "chaotic" we mean here that the invariant probability μ of the base transformation is assumed to be hyperbolic and to have local product structure: it is locally equivalent to a product of two measures, respectively, along stable and unstable sets.

Under additional assumptions, one can even prove that all Lyapunov exponents have multiplicity 1 outside an infinite-codimension subset. This follows from extensions of the Guivarc'h–Raugi criterion for certain linear cocycles over chaotic transformations, obtained by A Avila, C Bonatti, and M Viana.

Strange Attractors

This expression was coined by D Ruelle and F Takens in their celebrated study on the nature of fluid turbulence. E Hopf and also L D Landau and E M Lifshitz had suggested that turbulent motion arises from the existence in the phase space of invariant tori carrying quasiperiodic flows with large number of frequencies. Ruelle and Takens observed that dissipative systems such as viscous fluids do not generally have such quasiperiodic tori, and concluded that turbulence must be credited to a different mechanism: the presence of some "strange" attractor.

While they did not propose a precise definition, two main features were mentioned:

1. *Complex geometry*: a strange attractor is not reduced to an equilibrium point or a periodic solution of the system and, generally, should have a fractal structure.
2. *Chaotic dynamics*: solutions accumulating on the attractor should be sensitive to their initial states.

As more examples were found, it became apparent that the above two features do not always come together. This led to two types of definitions in the literature, depending on whether one emphasizes the geometry or the dynamics. We adopt the second point of view, and propose to define the strange attractor as one carrying an invariant ergodic physical measure which has some positive Lyapunov exponent. The notion of physical measure will be

defined near the end. The condition on the Lyapunov exponent ensures that the dynamics near the attractor is (exponentially) sensitive to the initial states.

Lorenz-Like Attractors

The uniformly hyperbolic attractors introduced by S Smale provided an interesting class of examples of strange attractors, both chaotic and fractal. Perhaps more striking, given that they originated from a concrete problem in fluid dynamics, were the strange attractors introduced by E N Lorenz. The Lorenz system of differential equations,

$$\begin{aligned} \dot{x} &= -\sigma x + \sigma y, \qquad & \sigma &= 10 \\ \dot{y} &= rx - y - xz, \qquad & r &= 28 \\ \dot{z} &= xy - bz, \qquad & b &= 8/3 \end{aligned} \qquad [12]$$

was derived from Lord Rayleigh's model for thermal convection, by Fourier expansion of the stream function and temperature, and truncation of all but three modes. Lorenz observed that its solutions depend sensitively on their initial states. Consequently, predictions based on the numerical integration of the equations may turn out to be very inaccurate, given that the initial data obtained from experimental measurements are never completely precise. This remarkable observation brought the issue of predictability in deterministic systems to a whole new light and motivated intense investigation of this and many other chaotic systems.

The dynamical behavior of the eqns [12] was first interpreted through certain geometric models where the presence of strange attractors, both chaotic and fractal, could be proved rigorously. It was much harder to prove that the original eqns [12] themselves have such an attractor. This was achieved just a few years ago, by W Tucker, by means of a computer-assisted rigorous argument. At about the same time, a mathematical theory of Lorenz-like attractors in three-dimensional space was developed by C Morales, M J Pacifico, and E Pujals. In particular, this theory shows that uniformly hyperbolic attractors and Lorenz-like attractors are the only ones which are robust under all small modifications of the vector field.

Hénon-Like Attractors

Starting from the work of Lorenz, many models of strange attractors have been found and described to some extent, often related to concrete problems. From a mathematical point of view, it is usually hard to give even a rough description of the dynamics in the chaotic regime. However, this was especially successful for the family of strange attractors introduced by M Hénon. He considered a very simple nonlinear system, particularly suited for numerical experimentation: the transformation

$$f(x,y) = (1 - ax^2 + by, x) \qquad [13]$$

where a and b are constant parameters. In a breakthrough, M Benedicks and L Carleson were able to prove that, for a set of parameter values with positive probability, this transformation has some nonhyperbolic attractor such that the orbits accumulating on it are sensitive to the starting point. The system [13] is also a model for many other situations, including the phenomenon of creation of homoclinic motions as parameters unfold, and the conclusions of Benedicks and Carleson have been extended to such situations, starting from the work of L Mora and M Viana.

Moreover, a detailed theory of Hénon-like attractors has been developed by M Benedicks, M Viana, D Wang, L S Young, and other authors. It follows from this theory that these attractors carry an invariant ergodic probability measure μ which describes the statistical behavior of almost all trajectories $f^j(x), j \geq 1$, that accumulate the attractor:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} \varphi(f^j(x)) = \int \varphi \, d\mu$$

for any continuous function φ. This property implies that, despite the fact that it is supported on a zero-volume set, the measure μ is, in some sense, physically observable. For this reason, one calls it a physical measure. In other words, time averages along typical orbits in the domain of attraction coincide with the space averages determined by the probability μ. Another property with physical relevance is that μ is the zero-noise limit of the stationary measures associated to the Markov chains obtained by adding random noise to f. One says that the system (f, μ) is stochastically stable.

See also: Chaos and Attractors; Dissipative Dynamical Systems of Infinite Dimension; Ergodic Theory; Fractal Dimensions in Dynamics; Generic Properties of Dynamical Systems; Gravitational *N*-Body Problem (Classical); Homoclinic Phenomena; Hyperbolic Dynamical Systems; Lagrangian Dispersion (Passive Scalar); Nonequilibrium Statistical Mechanics: Interaction between Theory and Numerical Simulations; Random Dynamical Systems; Synchronization of Chaos.

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Macroscopic Fluctuations and Thermodynamic Functionals

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Introduction

There is no theory so far of irreversible processes that is of the same generality as equilibrium statistical mechanics and presumably it may not exist. While in equilibrium the Gibbs distribution provides all the information and no equation of motion has to be solved, the dynamics plays the major role in nonequilibrium. The theory illustrated below refers to stationary states that are not restricted to being close to equilibrium, and for a wide class of models it can be shown to be exact. In this case one begins to see the appearance of some general principles.

In equilibrium statistical mechanics, there is a well-defined relationship, established by Boltzmann, between the probability of a state and its entropy. This fact was exploited by Einstein to study thermodynamic fluctuations. When we are out of equilibrium, for example, in a stationary state of a system in contact with two reservoirs, it is not completely clear how to define thermodynamic quantities such as the entropy or the free energy. One possibility is to use fluctuation theory to define their nonequilibrium analogs. In fact in this way, extensive quantities can be obtained, although not necessarily simply additive due to the presence of long-range correlations which seem to be a rather generic feature of nonequilibrium. This possibility has been pursued in recent years leading to a considerable number of interesting results. One can recognize two main lines.

1. Exact calculations in simplified models. This is well exemplified by the work of Derrida *et al.* (2002).
2. A general treatment of a class of continuous time Markov chains for which the simplified models provide examples. This is the point of view developed by Bertini *et al.* (2002, 2004).

Both approaches have been very effective and of course give the same results when a comparison is possible. The second approach seems to encompass a wide class of systems and has the advantage of leading to equations which apply to very different situations. This is the point of view we shall adopt in the following. The question whether there are alternative more natural ways of defining nonequilibrium entropies or free energies is, for the moment, open.

Boltzmann–Einstein Formula

The Boltzmann–Einstein theory of equilibrium thermodynamic fluctuations, as described for example in the book *Physique Statistique* by Landau–Lifshitz, states that the probability of a fluctuation from equilibrium in a macroscopic region of fixed volume V is proportional to $\exp\{V\Delta S/k\}$, where ΔS is the variation of entropy density in the region calculated along a reversible transformation creating the fluctuation and k is the Boltzmann constant.

This formula was derived by Einstein simply by inverting the Boltzmann relationship between entropy and probability. He considered this relationship as a phenomenological definition of the probability of a state.

Einstein theory refers to fluctuations from an equilibrium state, that is from a stationary state of a system isolated or in contact with reservoirs characterized by the same chemical potentials so that there is no flow of heat, electricity, chemical substances, etc., across the system. When in contact with reservoirs, ΔS is the variation of the total entropy (system + reservoirs) which, for fluctuations of constant volume and temperature, is equal to $-\Delta F/T$, where ΔF is the variation of the free energy of the system and T the temperature. In the following, we refer to $\Delta F/T$, our main object of study, as the entropy and use the letter S for it but no confusion should arise.

The important question we address is then: what happens if the system is stationary but not in equilibrium, that is, flows of physical quantities are present due to external fields and/or different chemical potentials at the boundaries? To start with it is not always clear whether a closed macroscopic dynamical description is possible. If the system admits such a description of the kind provided by hydrodynamic

equations, a fact which can be rigorously established in simplified models, a reasonable goal is to find an explicit connection between time-independent thermodynamic quantities (e.g., the entropy) and dynamical macroscopic properties (e.g., transport coefficients). As we shall see, the study of large fluctuations provides such a connection. It leads in fact to a dynamical theory of the entropy which is shown to satisfy a Hamilton–Jacobi equation (HJE) in infinitely many variables requiring the transport coefficients as input. Its solution is straightforward in the case of homogeneous equilibrium states and highly nontrivial in stationary nonequilibrium states (SNSs). In the first case we recover a well-known relationship widely used in the physical and physico-chemical literature. There are several one-dimensional models, where the HJE reduces to a nonlinear ordinary differential equation which, even if it cannot be solved explicitly, leads to the important conclusion that the nonequilibrium entropy is a nonlocal functional of the thermodynamic variables. This implies that correlations over macroscopic scales are present. The existence of long-range correlations is probably a generic feature of SNSs and more generally of situations where the dynamics is not time-reversal invariant. As a consequence if we divide a system into two subsystems, the entropy is not necessarily simply additive.

The first step toward the definition of a nonequilibrium entropy is the study of fluctuations in macroscopic evolutions described by hydrodynamic equations. In a dynamical setting, a typical question one may ask is the following: what is the most probable trajectory followed by the system in the spontaneous emergence of a fluctuation or in its relaxation to an equilibrium or a stationary state? To answer this question, one first derives a generalized Boltzmann–Einstein formula from which the most probable trajectory can be calculated by solving a variational principle. The entropy is related to the logarithm of the probability of such a trajectory and satisfies the HJE associated to the variational principle.

For states near equilibrium, an answer to this type of questions was given by Onsager and Machlup in 1953. The Onsager–Machlup theory gives the following result under the assumption of time reversibility of the microscopic dynamics. In the situation of a linear hydrodynamic equation and small fluctuations, that is, close to equilibrium, the most probable creation and relaxation trajectories of a fluctuation are time reversals of one another. This conclusion holds also in nonlinear hydrodynamic regimes and without the assumption of small fluctuations. This follows from the study of concrete models. In SNSs, on the other hand, time-reversal invariance is broken and the creation and relaxation trajectories of a fluctuation are not time reversals of one another.

In the following we refer to boundary-driven stationary nonequilibrium states, for example, a thermodynamic system in contact with reservoirs characterized by different temperatures and chemical potentials, but there is no difficulty in including an external field acting in the bulk.

Microscopic and Macroscopic Dynamics

We consider many-body systems in the limit of infinitely many degrees of freedom. The basic general assumption of the theory is Markovian evolution. Microscopically, we assume that the evolution is described by a Markov process X_τ which represents the state of the system at time τ. This hypothesis probably is not so restrictive, because the dynamics of Hamiltonian systems interacting with thermostats finally is also reduced to the analysis of a Markov process. Several examples are discussed in the literature. To be more precise, X_τ represents the set of variables necessary to specify the state of the microscopic constituents interacting among themselves and with the reservoirs. The SNS is described by a stationary, that is, invariant with respect to time shifts, probability distribution P_{st} over the trajectories of X_τ.

Macroscopically, the usual interpretation of Markovian evolution is that the time derivatives of thermodynamic variables $\dot{\rho}_i$ at a given instant of time depend only on the ρ_i's and the affinities (thermodynamic forces) $\partial S/\partial \rho_i$ at the same instant of time. Our next assumption can then be formulated as follows: the system admits a macroscopic description in terms of density fields which are the local thermodynamic variables. For simplicity of notation, we assume that there is only one thermodynamic variable (e.g., ρ, the density). The evolution of the field $\rho = \rho(t, u)$, where t and u are the macroscopic time and space coordinates (see below), is given by diffusion-type hydrodynamic equations of the form

$$\begin{aligned} \partial_t \rho &= \tfrac{1}{2}\nabla \cdot (D(\rho)\nabla\rho) \\ &= \tfrac{1}{2} \sum_{1\le i,j\le d} \partial_{u_i}\left(D_{i,j}(\rho)\partial_{u_j}\rho\right) \\ &= \mathcal{D}(\rho) \end{aligned} \qquad [1]$$

The interaction with the reservoirs appears as boundary conditions to be imposed on solutions of [1]. We assume that there exists a unique stationary solution $\bar{\rho}$ of [1], that is, a profile $\bar{\rho}(u)$, which satisfies the appropriate boundary conditions and is such that $\mathcal{D}(\bar{\rho}) = 0$. This holds if the diffusion matrix $D_{i,j}(\rho)$ in [1] is strictly elliptic, namely there exists a constant $c > 0$ such that $D(\rho) \ge c$ (in matrix sense).

These equations derive from the underlying microscopic dynamics through an appropriate

scaling limit in which the microscopic time and space coordinates τ, x are rescaled as follows: $t = \tau/N^2, u = x/N$, where N represents the linear size of the system. For lattice systems, N is an integer. The hydrodynamic equation [1] represents a law of large numbers with respect to the probability measure $P_{\rm st}$ conditioned on an initial state X_0. The initial conditions for [1] are determined by X_0. Of course, many microscopic configurations give rise to the same value of $\rho(0,u)$. In general, $\rho = \rho(t,u)$ is an appropriate limit of a local observable $\rho_N(X_\tau)$ as the number N of degrees of freedom diverges.

The hypothesis of Markovian evolution is also the basis of the 1931 Onsager's theory of irreversible processes near equilibrium. Onsager, however, did not rely on any microscopic model and assumed, near the equilibrium, linear hydrodynamic equations or regression equations as he called them. His equations, ignoring space dependence, were of the form

$$\dot{\rho}_i = -\sum_i D_{ij}\rho_j \qquad [2]$$

The diffusion matrix D is related to Onsager transport matrix χ and the entropy by the relationship

$$D = \chi s \qquad [3]$$

where the elements of s are $\partial^2 S/\partial\rho_i\partial\rho_j$. The matrix χ is defined by the relationship between flows and affinities

$$\dot{\rho}_i = -\sum_i \chi_{ij}\frac{\partial S}{\partial \rho_j} \qquad [4]$$

The indices ij here label different thermodynamic variables. The matrix χ is symmetric, a property known as Onsager reciprocity. Equations [2] and [3] follow by developing the entropy near an equilibrium state, that is, by taking a quadratic expression as an approximation. The minus sign in eqn [4] is due to our convention in which the entropy has the same sign as the free energy.

Equation [3] permits to reconstruct the entropy from the knowledge of the coefficients D and χ and has been widely used especially in physical chemistry. In SNSs, eqn [3] is replaced by a Hamilton–Jacobi-type equation for the entropy.

Dynamical Boltzmann–Einstein Formula

The basic assumption is that the stationary ensemble $P_{\rm st}$ admits a principle of large deviations describing the fluctuations of the thermodynamic variables appearing in the hydrodynamic equation. This means the following. The probability that for large N, the evolution of the random variable ρ_N deviates from the solution of the hydrodynamic equation and is close to some trajectory $\hat{\rho}(t)$ is exponentially small and of the form

$$\begin{aligned} P_{\rm st}(\rho_N(X_{N^2t}) \sim \hat{\rho}(t), t \in [t_1, t_2]) \\ \approx e^{-N^d[S(\hat{\rho}(t_1)) + J_{[t_1,t_2]}(\hat{\rho})]} \\ = e^{-N^d I_{[t_1,t_2]}(\hat{\rho})} \end{aligned} \qquad [5]$$

where d is the dimensionality of the system, $J(\hat{\rho})$ is a functional which vanishes if $\hat{\rho}(t)$ is a solution of [1] and $S(\hat{\rho}(t_1))$ is the entropy cost to produce the initial density profile $\hat{\rho}(t_1)$. We normalize S so that $S(\bar{\rho}) = 0$. Therefore, $J(\hat{\rho})$ represents the extra cost necessary to follow the trajectory $\hat{\rho}(t)$. Finally, $\rho_N(X_{N^2t}) \sim \hat{\rho}(t)$ means closeness in some metric and $\approx$ denotes logarithmic equivalence as $N \to \infty$. Equation [5] is the dynamical generalization of the Boltzmann–Einstein formula. Experience with many models justifies this assumption.

To understand how [5] leads to a dynamical theory of the entropy, we discuss its properties under time reversal. Let us denote by θ the time inversion operator defined by $\theta X_\tau = X_{-\tau}$. The probability measure $P^*_{\rm st}$ describing the evolution of the time-reversed process X^*_τ is given by the composition of $P_{\rm st}$ and θ^{-1}, that is,

$$\begin{aligned} P^*_{st}(X^*_\tau = \phi_\tau, \tau \in [\tau_1, \tau_2]) \\ = P_{st}(X_\tau = \phi_{-\tau}, \tau \in [-\tau_2, -\tau_1]) \end{aligned} \qquad [6]$$

Let L be the generator of the microscopic dynamics. We remind that L induces the evolution of observables (functions on the state space) according to the equation $\partial_\tau E_{X_0}[f(X_\tau)] = E_{X_0}[(Lf)(X_\tau)]$, where E_{X_0} stands for the expectation with respect to $P_{\rm st}$ conditioned on the initial state X_0.

The time-reversed dynamics, that is, the dynamics which inverts the direction of the fluxes through the system, for example, heat flows under this dynamics from lower to higher temperatures, is generated by the adjoint L^* of L with respect to the invariant measure μ:

$$E^\mu[fLg] = E^\mu[(L^*f)g] \qquad [7]$$

The measure μ, which is the same for both processes, is a distribution over the configurations of the system and formally satisfies $\mu L = 0$. The expectation with respect to μ is denoted by E^μ and f, g are observables. We note that the probability $P_{\rm st}$, and therefore $P^*_{\rm st}$, depends on the invariant measure μ. The finite-dimensional distributions of $P_{\rm st}$ are in fact given by

$$\begin{aligned} P_{\rm st}(X_{\tau_1} = \phi_{\tau_1}, \ldots, X_{\tau_n} = \phi_{\tau_n}) \\ = \mu(\phi_{\tau_1})\, p_{\tau_2-\tau_1}(\phi_{\tau_1} \to \phi_{\tau_2}) \cdots p_{\tau_n-\tau_{n-1}}(\phi_{\tau_{n-1}} \to \phi_{t\tau_n}) \end{aligned} \qquad [8]$$

where $p_\tau(\phi_1 \to \phi_2)$ is the transition probability. According to [6] the finite-dimensional distributions of P^*_{st} are

$$P^*_{st}\left(X^*_{\tau_1} = \phi_{\tau_1}, \ldots, X^*_{\tau_n} = \phi_{\tau_n}\right) = \mu(\phi_{\tau_1})\, p^*_{\tau_2-\tau_1}(\phi_{\tau_1} \to \phi_{\tau_2}) \cdots p^*_{\tau_n-\tau_{n-1}}(\phi_{\tau_{n-1}} \to \phi_{t\tau_n}) = \mu(\phi_{\tau_n}) p_{\tau_n-\tau_{n-1}}(\phi_{\tau_n} \to \phi_{\tau_{n-1}}) \cdots p_{\tau_2-\tau_1}(\phi_{\tau_2} \to \phi_{\tau_1}) \quad [9]$$

In particular, the transition probabilities $p_\tau(\phi_1 \to \phi_2)$ and $p_\tau{}^*(\phi_1 \to \phi_2)$ are related by

$$\mu(\phi_1)\, p_\tau(\phi_1 \to \phi_2) = \mu(\phi_2)\, p_\tau{}^*(\phi_2 \to \phi_1) \quad [10]$$

This relationship reduces to the well-known detailed balance condition if $p_\tau(\phi_1 \to \phi_2) = p_\tau{}^*(\phi_1 \to \phi_2)$.

We require that also the evolution generated by L^* admits a hydrodynamic description, that we call the adjoint hydrodynamics, which, however, is not necessarily of the same form as [1]. In fact, we consider models in which the adjoint hydrodynamics is nonlocal in space.

In order to avoid confusion, we emphasize that what is usually called an equilibrium state for a reversible dynamics, as distinguished from an SNS, corresponds to the special case $L^* = L$, that is, the detailed balance principle holds. In such a case, P_{st} is invariant under time reversal and the two hydrodynamics coincide.

We now derive a first consequence of our assumptions, that is, the relationship between the functionals I and I^* associated to the dynamics L and L^* by [5]. From eqn [6], it follows that

$$I^*_{[t_1,t_2]}(\hat{\rho}) = I_{[-t_2,-t_1]}(\theta\hat{\rho}) \quad [11]$$

with obvious notations. More explicitly, this equation reads

$$S(\hat{\rho}(t_1)) + J^*_{[t_1,t_2]}(\hat{\rho}) = S(\hat{\rho}(t_2)) + J_{[-t_2,-t_1]}(\theta\hat{\rho}) \quad [12]$$

where $\hat{\rho}(t_1), \hat{\rho}(t_2)$ are the initial and final points of the trajectory and $S(\hat{\rho}(t_i))$ the entropies associated with the creation of the fluctuations $\hat{\rho}(t_i)$ starting from the SNS. The functional J^* vanishes on the solutions of the adjoint hydrodynamics. To compute J^*, it is necessary to know the entropy S.

We consider now the following physical situation. The system is macroscopically in the stationary state $\bar{\rho}$ at $t = -\infty$, but at $t = 0$ we find it in the state ρ. We want to determine the most probable trajectory followed in the spontaneous creation of this fluctuation. According to [5], this trajectory is the one that minimizes J among all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ in the time interval $[-\infty, 0]$. From [12], recalling that $S(\bar{\rho}) = 0$, we have that

$$J_{[-\infty,0]}(\hat{\rho}) = S(\rho) + J^*_{[0,\infty]}(\theta\hat{\rho}) \quad [13]$$

The right-hand side is minimal if $J^*_{[0,\infty]}(\theta\hat{\rho}) = 0$, that is, if $\theta\hat{\rho}$ is a solution of the adjoint hydrodynamics. The existence of such a relaxation solution is due to the fact that the stationary solution $\bar{\rho}$ is attractive also for the adjoint hydrodynamics. We have therefore the following consequences:

> In a SNS the spontaneous emergence of a macroscopic fluctuation takes place most likely following a trajectory which is the time reversal of the relaxation path according to the adjoint hydrodynamics.

This implies that the entropy is related to J by

$$S(\rho) = \inf_{\hat{\rho}} J_{[-\infty,0]}(\hat{\rho}) \quad [14]$$

where the minimum is taken over all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ.

We note that the reversibility of the microscopic process X_τ, which we call microscopic reversibility, is not needed in order to deduce the Onsager–Machlup result (i.e., that the trajectory which creates the fluctuation is the time reversal of the relaxation trajectory). In fact, Onsager–Machlup result holds if and only if the hydrodynamics coincides with the adjoint hydrodynamics, which we call macroscopic reversibility. Indeed, it is possible to construct microscopic nonreversible models, $L \neq L^*$, in which the hydrodynamics and the adjoint hydrodynamics coincide.

Spontaneous fluctuations, including Onsager–Machlup time-reversal symmetry, have been observed in stochastically perturbed reversible electronic devices. In nonreversible systems, an asymmetry between the emergence and the relaxation of fluctuations has been observed. The above discussion provides the explanation.

The Hamilton–Jacobi Equation and Its Consequences

We assume that the functional J has a density (which plays the role of a Lagrangian), that is,

$$J_{[t_1,t_2]}(\hat{\rho}) = \int_{t_1}^{t_2} dt\,\mathcal{L}(\hat{\rho}(t), \partial_t\hat{\rho}(t)) \quad [15]$$

Let us introduce the Hamiltonian $\mathcal{H}(\rho, H)$ as the Legendre transform of $\mathcal{L}(\rho, \partial_t\rho)$, that is,

$$\mathcal{H}(\rho, H) = \sup_{\xi}\{\langle \xi, H\rangle - \mathcal{L}(\rho, \xi)\} \quad [16]$$

where $\langle \cdot, \cdot \rangle$ denotes integration with respect to the macroscopic space coordinates u.

Noting that $\mathcal{H}(\bar{\rho}, 0) = 0$, the Hamilton–Jacobi equation associated to [14] is

$$\mathcal{H}\left(\rho, \frac{\delta S}{\delta \rho}\right) = 0 \qquad [17]$$

This is an equation for the functional derivative $C(\rho) = \delta S/\delta\rho$, but not all the solutions of the equation $\mathcal{H}(\rho, C(\rho)) = 0$ are the derivatives of some functional. Of course, only those which are the derivative of a functional are relevant for us.

We now specify the Hamilton–Jacobi equation [17] for boundary-driven lattice gases. For models with purely diffusive hydrodynamics [1], we expect a quadratic large deviation functional of the form

$$J_{[t_1,t_2]}(\hat{\rho}) = \frac{1}{2}\int_{t_1}^{t_2} dt \langle \nabla^{-1}(\partial_t\hat{\rho} - \mathcal{D}(\rho)), \chi(\hat{\rho})^{-1}\nabla^{-1}(\partial_t\hat{\rho} - \mathcal{D}(\rho))\rangle \qquad [18]$$

where $\mathcal{D}(\rho)$ is the right-hand side of the hydrodynamic equation [1], and by $\nabla^{-1}f$ we mean a vector field whose divergence equals f. The form [18], which can be derived for several models, is expected to be very general: the functional $J(\hat{\rho})$ measures how much $\hat{\rho}$ differs from a solution of the hydrodynamics [1]. The matrix $\chi(\rho) = \chi(\rho)$ with $\chi(\rho)$ has the same role in our more general context, as the Onsager matrix in [4]. This form of J is also typical for diffusion processes described by finite-dimensional Langevin equations (Freidlin–Wentzell theory).

In this case, the Lagrangian $\mathcal{L}$ is quadratic in $\partial_t\hat{\rho}(t)$ and the associated Hamiltonian is given by

$$\mathcal{H}(\rho, H) = \tfrac{1}{2}\langle \nabla H, \chi(\rho)\nabla H\rangle + \langle H, \mathcal{D}(\rho)\rangle \qquad [19]$$

so that the Hamilton–Jacobi equation [17] takes the form

$$\frac{1}{2}\left\langle \nabla\frac{\delta S}{\delta\rho}, \chi(\rho)\nabla\frac{\delta S}{\delta\rho}\right\rangle + \left\langle \frac{\delta S}{\delta\rho}, \mathcal{D}(\rho)\right\rangle = 0 \qquad [20]$$

As is well known in mechanics, the Hamilton–Jacobi equation has many solutions and we must give a criterion to select the correct one. The criterion which the correct solution has to satisfy is that it must be a Lyapunov function with respect to the unique stationary state.

It is a simple calculation to show that eqn [3] follows from HJE, if we look for a solution which is a local function of ρ. This is the right choice in equilibrium where correlations over macroscopic distances are not expected if the microscopic forces are short range.

Out of equilibrium, it has been shown by direct calculation that for a special model, the symmetric simple exclusion, the entropy is a nonlocal function of the thermodynamic variables, that is, space correlations extend to macroscopic distances. This result can be derived in a simple way from HJE as we will discuss later.

Lattice gases which do not conserve the number of particles do not give rise in general to a purely diffusive hydrodynamics but rather to a reaction diffusion equation. In this case, the large deviation functional will not have the quadratic form [18] and also the HJE will not be quadratic. An example in which particles can be created and destroyed is the so-called Kawasaki–Glauber dynamics. In this case, HJE has exponential nonlinearities.

Nonequilibrium Fluctuation Dissipation Relation

We now derive a twofold generalization of the celebrated fluctuation dissipation relationship: it is valid in nonequilibrium states and in nonlinear regimes.

Such a relationship will hold provided the rate function J^* of the time-reversed process is of the form [18] with $\mathcal{D}$ replaced by $\mathcal{D}^*$, the adjoint hydrodynamics,

$$\partial_t\rho = \mathcal{D}^*(\rho) \qquad [21]$$

with the same boundary conditions as [1].

If J^* has the form

$$J^*_{[t_1,t_2]}(\hat{\rho}) = \frac{1}{2}\int_{t_1}^{t_2} dt \langle (\nabla^{-1}(\partial_t\hat{\rho} - \mathcal{D}^*(\hat{\rho})), \chi(\hat{\rho})^{-1}\nabla^{-1}(\partial_t\hat{\rho} - \mathcal{D}^*(\hat{\rho}))\rangle \qquad [22]$$

by taking the variation of eqn [12], we get

$$\mathcal{D}(\rho) + \mathcal{D}^*(\rho) = \nabla\cdot\left(\chi(\rho)\nabla\frac{\delta S}{\delta\rho}\right) \qquad [23]$$

This relation can be verified explicitly for the nonequilibrium zero-range process which we discuss later and holds for several other models. It is also easy to check that the linearization of [23] around the stationary profile $\bar{\rho}$ yields a fluctuation dissipation relationship which reduces to the usual one in equilibrium.

The fluctuation dissipation relation [23] can be used to obtain the adjoint hydrodynamics from $\mathcal{D}(\rho)$ and $\delta S/\delta\rho$; the first is usually known and the second can be calculated from the Hamilton–Jacobi equation.

H Theorem

We show that the functional S is decreasing along the solutions of both the hydrodynamic equation [1] and the adjoint hydrodynamics

$$\partial_t\rho = \mathcal{D}^*(\rho) = \nabla\cdot\left(\chi(\rho)\nabla\frac{\delta S}{\delta\rho}\right) - \mathcal{D}(\rho) \qquad [24]$$

Let $\rho(t)$ be a solution of [1] or [24]; by using the Hamilton–Jacobi equation [20], we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}S(\rho(t)) &= \left\langle \frac{\delta S}{\delta \rho}(\rho(t)), \partial_t \rho(t) \right\rangle \\ &= -\frac{1}{2}\left\langle \nabla \frac{\delta S}{\delta \rho}(\rho(t)), \chi(\rho(t))\nabla \frac{\delta S}{\delta \rho}(\rho(t)) \right\rangle \\ &\leq 0 \end{aligned} \qquad [25]$$

In particular, we have that $(\mathrm{d}/\mathrm{d}t)S(\rho(t)) = 0$ if and only if $(\delta S/\delta \rho)(\rho(t)) = 0$.

We remark that the right-hand side of [25] vanishes in the stationary state, that is, there is no internal entropy production due to the evolution. On the other hand, there is a steady entropy production due to the differences in the chemical potentials of the reservoirs. This is not discussed in this article.

Decomposition of Hydrodynamics

There is a structural property of hydrodynamics which follows from the HJE. The hydrodynamic equation can be decomposed as the sum of a gradient vector field and a vector field $\mathcal{A}$ orthogonal to it in the metric induced by the operator K^{-1}, where $Kf = -\nabla \cdot (\chi(\rho)\nabla f)$, namely

$$\mathcal{D}(\rho) = \frac{1}{2}\nabla \cdot \left(\chi(\rho)\nabla \frac{\delta S}{\delta \rho}\right) + \mathcal{A}(\rho) \qquad [26]$$

with

$$\left\langle K\frac{\delta S}{\delta \rho}, K^{-1}\mathcal{A}(\rho)\right\rangle = \left\langle \frac{\delta S}{\delta \rho}, \mathcal{A}(\rho)\right\rangle = 0$$

Similarly, using the fluctuation dissipation relationship [23] for the adjoint hydrodynamics, we have

$$\mathcal{D}^*(\rho) = \frac{1}{2}\nabla \cdot \left(\chi(\rho)\nabla \frac{\delta S}{\delta \rho}\right) - \mathcal{A}(\rho) \qquad [27]$$

Since $\mathcal{A}$ is orthogonal to $\delta S/\delta \rho$, it does not contribute to the entropy production. The vector field $\mathcal{A}$ is odd under time reversal like a magnetic force.

Both terms of the decomposition vanish in the stationary state, that is, when $\rho = \bar{\rho}$. Whereas in equilibrium the hydrodynamics is the gradient flow of the entropy S, the term $\mathcal{A}(\rho)$ is characteristic of nonequilibrium states. Note that, for small fluctuations $\rho \approx \bar{\rho}$, small differences in the chemical potentials at the boundaries, $\mathcal{A}(\rho)$ becomes a second-order quantity and Onsager theory is a consistent approximation.

Equation [26] is interesting because it separates the dissipative part of the hydrodynamic evolution associated to the thermodynamic force $\delta S/\delta \rho$ and provides therefore an important physical information. Notice that the thermodynamic force $\delta S/\delta \rho$ appears linearly in the hydrodynamic equation even when this is nonlinear in the macroscopic variables.

In general, the two terms of the decomposition [26] are nonlocal in space even if $\mathcal{D}$ is a local function of ρ. This is the case for the simple exclusion process discussed later. Furthermore while the form of the hydrodynamic equation does not depend explicitly on the chemical potentials, $\delta S/\delta \rho$ and $\mathcal{A}$ do.

To understand how the decomposition [26] arises microscopically, let us consider a stochastic lattice gas. Let

$$L = \tfrac{1}{2}(L + L^*) + \tfrac{1}{2}(L - L^*) \qquad [28]$$

be its Markov generator, where L^* is the adjoint of L with respect to the invariant measure, namely the generator of the time-reversed microscopic dynamics. The term $L - L^*$ behaves like a Liouville operator, that is, it is anti-Hermitian and, in the scaling limit, produces the term $\mathcal{A}$ in the hydrodynamic equation. This can be verified explicitly in the boundary-driven zero-range model introduced in the next section.

Since the adjoint generator can be written as $L^* = (L + L^*)/2 - (L - L^*)/2$, the adjoint hydrodynamics must be of the form [27]. In particular, if the microscopic generator is self-adjoint, we get $\mathcal{A} = 0$ and thus $\mathcal{D}(\rho) = \mathcal{D}^*(\rho)$. On the other hand, it may happen that microscopic nonreversible processes, namely for which $L \neq L^*$, can produce macroscopic reversible hydrodynamics if $L - L^*$ does not contribute to the hydrodynamic limit.

The decompositions [26] and [27] remind of the electrical conduction in the presence of a magnetic field. Consider the motion of electrons in a conductor: a simple model is given by the effective equation

$$\dot{\boldsymbol{p}} = -e\left(\boldsymbol{E} + \frac{1}{mc}\boldsymbol{p} \wedge \boldsymbol{H}\right) - \frac{1}{\tau}\boldsymbol{p} \qquad [29]$$

where $\boldsymbol{p}$ is the momentum, e the electron charge, $\boldsymbol{E}$ the electric field, $\boldsymbol{H}$ the magnetic field, m the mass, c the velocity of the light, and τ the relaxation time. The dissipative term $\boldsymbol{p}/\tau$ is orthogonal to the Lorentz force $\boldsymbol{p} \wedge \boldsymbol{H}$. We define time reversal as the transformation $\boldsymbol{p} \mapsto -\boldsymbol{p}, \boldsymbol{H} \mapsto -\boldsymbol{H}$. The adjoint evolution is given by

$$\dot{\boldsymbol{p}} = e\left(\boldsymbol{E} + \frac{1}{mc}\boldsymbol{p} \wedge \boldsymbol{H}\right) - \frac{1}{\tau}\boldsymbol{p} \qquad [30]$$

where the signs of the dissipation and the electromagnetic force transform in analogy to [26] and [27].

Let us consider in particular the Hall effect where we have conduction along a rectangular plate immersed in a perpendicular magnetic field H with a potential difference across the longer side. The magnetic field determines a potential difference across the other side of the plate. In our setting on the contrary, it is the difference in chemical potentials at the boundaries that introduces in the equations a "magnetic-like" term. There is therefore a kind of equivalence between certain externally applied fields and driving the system at the boundaries.

Minimum Dissipation Principle

In 1931 Onsager formulated, within his near equilibrium theory, a variational principle which shows that the hydrodynamic evolution minimizes at each instant of time a quadratic functional of $\dot{\rho}$. He called this the "minimum dissipation principle." We now show that the decomposition of the previous subsection leads to a natural exact generalization of this principle. We want to construct a functional of the variables ρ and $\dot{\rho}$ such that the Euler equation associated to the vanishing of the first variation under arbitrary changes of $\dot{\rho}$ is the hydrodynamic equation [1]. We define the "dissipation function"

$$F(\rho,\dot{\rho}) = \langle(\dot{\rho} - \mathcal{A}(\rho)), K^{-1}(\dot{\rho} - \mathcal{A}(\rho))\rangle \qquad [31]$$

and the functional

$$\begin{aligned}\Phi(\rho,\dot{\rho}) &= \dot{S}(\rho) + F(\rho,\dot{\rho}) \\ &= \left\langle \frac{\delta S}{\delta\rho}, \dot{\rho} \right\rangle + \langle(\dot{\rho} - \mathcal{A}(\rho)), \\ &\qquad K^{-1}(\dot{\rho} - \mathcal{A}(\rho))\rangle \end{aligned} \qquad [32]$$

which generalize the corresponding Onsager's definitions (Onsager 1931a, b). The operator K has been defined in the previous subsection.

It is easy to verify that

$$\delta_{\dot{\rho}}\Phi = 0 \qquad [33]$$

is equivalent to the hydrodynamic equation [1]. Furthermore, a simple calculation gives

$$F|_{\dot{\rho}=\mathcal{D}(\rho)} = \frac{1}{4}\left\langle \nabla\frac{\delta S}{\delta\rho}, \chi(\rho)\nabla\frac{\delta S}{\delta\rho} \right\rangle \qquad [34]$$

that is, $2F$ on the hydrodynamic trajectories equals the entropy production rate as in Onsager's near equilibrium approximation.

The dissipation function for the adjoint hydrodynamics is obtained by changing the sign of $\mathcal{A}$ in [31].

Entropy and Optimal Control

There is an interesting interpretation of the entropy as a minimal cost to produce a fluctuation by externally acting on the system. The idea is to show that there exists a cost function which on the optimal control trajectory coincides with the entropy difference with respect to the stationary state.

We add an external perturbation v to the hydrodynamic equation

$$\partial_t\rho = \tfrac{1}{2}\nabla\cdot(D(\rho)\nabla\rho) + v = \mathcal{D}(\rho) + v \qquad [35]$$

We want to choose v so as to drive, with minimal cost, the system from its stationary state $\bar{\rho}$ to an arbitrary state ρ. A simple cost function is

$$\frac{1}{2}\int_{t_1}^{t_2} \mathrm{d}s\langle v(s), K^{-1}(\rho(s))v(s)\rangle \qquad [36]$$

where $\rho(s)$ is the solution of [35] and we recall that $K(\rho)f = -\nabla\cdot(\chi(\rho)\nabla f)$. More precisely, given $\rho(t_1) = \bar{\rho}$, we want to drive the system to $\rho(t_2) = \rho$ by an external field v which minimizes [36]. This is a standard problem in control theory. Let

$$\mathcal{V}(\rho) = \inf\frac{1}{2}\int_{t_1}^{t_2} \mathrm{d}s\langle v(s), K^{-1}(\rho(s))v(s)\rangle \qquad [37]$$

where the infimum is taken with respect to all fields v which drive the system to ρ in an arbitrary time interval $[t_1, t_2]$. The optimal field v can be obtained by solving the Bellman equation which reads

$$\min_v\left\{\frac{1}{2}\langle v, K^{-1}(\rho)v\rangle - \left\langle \mathcal{D}(\rho) + v, \frac{\delta\mathcal{V}}{\delta\rho}\right\rangle\right\} = 0 \qquad [38]$$

It is easy to express the optimal v in terms of $\mathcal{V}$; we get

$$v = K\frac{\delta\mathcal{V}}{\delta\rho} \qquad [39]$$

Hence, [38] now becomes

$$\frac{1}{2}\left\langle\frac{\delta\mathcal{V}}{\delta\rho}, K(\rho)\frac{\delta\mathcal{V}}{\delta\rho}\right\rangle + \left\langle\mathcal{D}(\rho), \frac{\delta\mathcal{V}}{\delta\rho}\right\rangle = 0 \qquad [40]$$

By identifying the cost functional $\mathcal{V}(\rho)$ with $S(\rho)$, eqn [40] coincides with the Hamilton–Jacobi equation [20].

By inserting the optimal v [39] in [35] and identifying $\mathcal{V}$ with S, we get that the optimal trajectory $\rho(t)$ solves the time-reversed adjoint hydrodynamics, namely

$$\partial_t\rho = -\mathcal{D}^*(\rho) \qquad [41]$$

The trajectory of the spontaneous emergence of a fluctuation coincides therefore with the trajectory of minimal cost for the optimal control. The optimal field v does not depend on the nondissipative part $\mathcal{A}$ of the hydrodynamics.

Models

The general theory will now be illustrated by briefly describing models where it has been successfully applied. We consider examples of different nature in order to emphasize the generality and flexibility of the point of view developed in the previous section.

We have chosen three examples in which the theory is used in different ways. The first one, the zero-range process, can be solved in a simple way so that the theory can be verified in detail. In the second one, the symmetric simple exclusion, we derive from the HJE a nonlinear ordinary differential equation first obtained by Derrida, Lebowitz, and Speer through a direct rather complex calculation. This equation implies the nonlocality of the entropy in the SNS of this model. The third model, the Kawasaki–Glauber dynamics, provides the illustration of two aspects. Nonlocality of the entropy, that is, long-range correlations, can appear in isolated equilibrium states if the microscopic dynamics is not time-reversal invariant. This means that long-range correlations as a signature of time-reversal violation are not restricted to SNSs. The second aspect to be underlined is the effectiveness of the HJE in a more complex case: in fact in this model, the number of particles is not conserved which leads to a very complicated structure of the HJE.

As a general comment, we emphasize that dynamics microscopically different but leading to the same macroscopic description, in particular the same hydrodynamics and large deviation functional, are indistinguishable for the theory which is purely macroscopic.

Zero Range

We consider the so-called zero-range process which models a nonlinear diffusion of a lattice gas. The model is described by a positive integer variable $\eta_\tau(x)$ representing the number of particles at site x and time τ of a finite lattice which for simplicity we assume one dimensional. The particles jump with rates $g(\eta(x))$ to one of the nearest-neighbor sites $x+1, x-1$ with probability 1/2. The function $g(k)$ is nondecreasing and $g(0)=0$. We assume that our system interacts with two reservoirs of particles in positions N and $-N$ with rates p_+ and p_-, respectively. This model can be solved exactly and the previous theory can be checked in full detail.

Let us introduce the macroscopic coordinates, time $t=\tau/N^2$ and space $u=x/N$. To describe the macroscopic dynamics, we introduce the empirical density

$$\rho_N(t,u) = \frac{1}{N}\sum_{x=-N}^{N} \eta_{N^2t}(x)\delta(u-x/N) \qquad [42]$$

where $\delta(u-x/N)$ is the Dirac δ. One can prove that in the limit $N \to \infty$, the empirical density [42] tends in probability to a continuous function $\rho_t(u)$, which satisfies the following hydrodynamic equation:

$$\partial_t \rho = \tfrac{1}{2}\Delta\phi(\rho) = \mathcal{D}(\rho) \qquad [43]$$

where $\phi(\rho)$ can be explicitly defined in terms of the rates $g(\eta)$. The boundary conditions for [43] are $\phi(\rho(t,\pm 1)) = p_\pm$.

The adjoint hydrodynamics is

$$\partial_t \rho = \frac{1}{2}\Delta\phi(\rho) - \alpha\nabla\left\{\frac{\phi(\rho)}{\lambda(u)}\right\} = \mathcal{D}^*(\rho) \qquad [44]$$

with

$$\lambda(u) = \frac{p_+ - p_-}{2}u + \frac{p_+ + p_-}{2}$$

and

$$\alpha = \frac{p_+ - p_-}{2}$$

The boundary conditions for [44] are the same as for [43]. The second term on the right-hand side of [44] is proportional to the difference of the chemical potentials and produces an inversion of the particle flux. The action functionals $J(\hat{\rho})$ and $J^*(\hat{\rho})$ for this model have been computed and have the form [18] and [22], respectively, with $\chi(\rho)=\phi(\rho)$. The entropy $S(\rho)$ can be easily computed directly from the expression of the invariant measure which is of product type and is known explicitly:

$$S(\rho) = \int_{-1}^{1} du \left[\rho(u)\log\frac{\phi(\rho(u))}{\lambda(u)} - \log\frac{Z(\phi(\rho(u)))}{Z(\lambda(u))}\right] \qquad [45]$$

where

$$Z(\phi) = 1 + \sum_{k=1}^{\infty} \frac{\phi^k}{g(1)\cdots g(k)}$$

It is easy to verify that it solves the HJE. Due to the special zero-range character of the interaction in this model, there are no long-range correlations in nonequilibrium states.

Simple Exclusion

The simple exclusion process is a model of a lattice gas with an exclusion principle: a particle can move to a neighboring site, with rate 1/2 for each side, only if this is empty. We consider again a one-dimensional case and we denote by $\eta_x(\tau) \in \{0, 1\}$ the number of particles at the site x at (microscopic) time τ. The system is in contact with particle reservoirs at the boundaries $\pm N$ where a particle is created with rates $p_\pm$ if the boundary site is empty and is destroyed $1 - p_\pm$ if it is occupied. In contrast to the zero-range model, the invariant measure carries long-range correlations making the entropy nonlocal.

The hydrodynamic equation for the simple exclusion process can be derived as for the zero-range process; in fact, it is easier in this case because a simple computation leads directly to a closed equation for the empirical density which is defined as in [42] except that the variable η now takes only the values 0 or 1. We find that the limiting density evolves according to the linear heat equation

$$\partial_t \rho(t, u) = \tfrac{1}{2}\Delta\rho(t, u) = \mathcal{D}(\rho) \qquad [46]$$

with boundary conditions

$$\rho(t, \pm 1) = \frac{p_\pm}{1 + p_\pm} = \rho_\pm$$

In this case, the density of particles ρ takes values in [0,1]. We use the HJE to calculate the entropy. For this model, we have $\chi(\rho) = \rho(1 - \rho)$. We show that the solution of the HJE for $S(\rho)$ (which is a functional derivative equation) can be reduced to the solution of an ordinary differential equation.

The Hamilton–Jacobi equation for the simple exclusion process is

$$\left\langle \nabla \frac{\delta S}{\delta \rho}, \rho(1 - \rho)\nabla \frac{\delta S}{\delta \rho}\right\rangle + \left\langle \frac{\delta S}{\delta \rho}, \Delta\rho \right\rangle = 0 \qquad [47]$$

We look for a solution of the form

$$\frac{\delta S}{\delta \rho(u)} = \log \frac{\rho(u)}{1 - \rho(u)} - \phi(u; \rho) \qquad [48]$$

for some functional $\phi(u; \rho)$ to be determined satisfying the boundary conditions

$$\phi(\pm 1) = \log \frac{\rho_\pm}{1 - \rho_\pm}$$

in the space variable. The first term on the right-hand side is the derivative of the equilibrium entropy, that is for boundary conditions $\rho_- = \rho_+$.

Inserting [48] into [47], we get (note that $\rho - e^\phi/(1 + e^\phi)$ vanishes at the boundary)

$$\begin{aligned}
0 &= -\left\langle \nabla\left(\log \frac{\rho}{1 - \rho} - \phi\right), \rho(1 - \rho)\nabla\phi \right\rangle \\
&= -\langle \nabla\rho, \nabla\phi\rangle + \left\langle \rho(1 - \rho), (\nabla\phi)^2 \right\rangle \\
&= -\left\langle \nabla\left(\rho - \frac{e^\phi}{1 + e^\phi}\right), \nabla\phi \right\rangle \\
&\quad - \left\langle \left(\rho - \frac{e^\phi}{1 + e^\phi}\right)\left(\rho - \frac{1}{1 + e^\phi}\right), (\nabla\phi)^2 \right\rangle \\
&= \left\langle \left(\rho - \frac{e^\phi}{1 + e^\phi}\right), \left(\Delta\phi + \frac{(\nabla\phi)^2}{1 + e^\phi} - \rho(\nabla\phi)^2\right) \right\rangle
\end{aligned}$$

We obtain a nontrivial solution of the Hamilton–Jacobi if we solve the following ordinary differential equation, corresponding to the vanishing of the right side of the scalar product, which relates the functional $\phi(u) = \phi(u; \rho)$ to ρ:

$$\begin{aligned}
&\frac{\Delta\phi(u)}{[\nabla\phi(u)]^2} + \frac{1}{1 + e^{\phi(u)}} = \rho(u), \quad u \in (-1, 1) \\
&\phi(\pm 1) = \log \frac{\rho_\pm}{1 - \rho_\pm}
\end{aligned} \qquad [49]$$

It is clear that ϕ is a nonlocal functional of ρ. A computation shows that the derivative of the functional

$$\begin{aligned}
S(\rho) = \int du \Big\{ &\rho \log \rho + (1 - \rho)\log(1 - \rho) \\
&+ (1 - \rho)\phi - \log(1 + e^\phi) + \log \frac{\nabla\phi}{\nabla\bar{\rho}} \Big\}
\end{aligned}$$

is given by [48] when $\phi(u; \rho)$ solves [49].

Kawasaki–Glauber Dynamics

The model consists of particles on a lattice evolving according to two basic dynamical processes:

1. a particle can move to a neighboring site if this is empty as in the simple exclusion and
2. a particle can disappear in an occupied site or be created if this is empty, the rate depending on the nearby configuration.

The first process is conservative while the second is not.

As before the object of our study is the empirical density [42]. It is possible to show that as N goes to infinity, $\rho(t, u)$ is a solution of

$$\partial_t \rho = \tfrac{1}{2}\Delta\rho + B(\rho) - D(\rho) \qquad [50]$$

with

$$B(\rho) = E_{\nu_\rho}(c(\eta)(1 - \eta(0))) \qquad [51]$$

$$D(\rho) = E_{\nu_\rho}(c(\eta)\eta(0)) \qquad [52]$$

where ν_ρ is the Bernoulli product distribution with parameter ρ. Typically, $B(\rho)$ and $D(\rho)$ are polynomials in ρ. For this model we consider equilibrium states so that we can take periodic boundary conditions. An equilibrium state corresponds to a density $\bar{\rho}$ which is the solution of the equation $B(\rho) = D(\rho)$ and gives a minimum of the potential $V(\rho) = \int^\rho [D(\rho') - B(\rho')]\mathrm{d}\rho'$. We admit potentials with several minima. The Hamiltonian associated to the large deviation functional for this model is not quadratic:

$$\begin{aligned}\mathcal{H}(\rho, H) = \int \mathrm{d}u\Big\{\frac{1}{2}H\Delta\rho + \frac{1}{2}(\nabla H)^2\rho(1-\rho) \\ - B(\rho)(1 - \exp H) - D(\rho) \\ \times (1 - \exp(-H))\Big\}\end{aligned} \qquad [53]$$

where H has the role of the conjugate momentum. The Hamilton–Jacobi equation

$$\mathcal{H}\left(\rho, \frac{\delta S}{\delta \rho}\right) = 0 \qquad [54]$$

is therefore very complicated but can be solved by successive approximations using as an expansion parameter $\rho - \bar{\rho}$, where $\bar{\rho}$ is a solution of $B(\rho) = D(\rho)$ that is a stationary solution of hydrodynamics. For $\rho = \bar{\rho}$, we have $\delta S/\delta\rho = 0$. We are looking for an approximate solution of [54] of the form

$$\begin{aligned}S(\rho) = \frac{1}{2}\int \mathrm{d}u \int \mathrm{d}v(\rho(u) - \bar{\rho})k(u,v)(\rho(v) - \bar{\rho}) \\ + o(\rho - \bar{\rho})^2\end{aligned} \qquad [55]$$

The kernel $k(u,v)$ is the inverse of the density correlation function $c(u,v)$.

$$\int c(u,y)k(y,v)\,\mathrm{d}y = \delta(u - v) \qquad [56]$$

By inserting [55] in [54], one can show that $k(u,v)$ satisfies the following equation:

$$\begin{aligned}\tfrac{1}{2}\bar{\rho}(1-\bar{\rho})\Delta_u k(u,v) - b_0 k(u,v) \\ - \tfrac{1}{2}\Delta_u \delta(u-v) + (d_1 - b_1)\delta(u-v) = 0\end{aligned} \qquad [57]$$

where

$$b_1 = B'(\rho)|_{\rho=\bar{\rho}}, \qquad d_1 = D'(\rho)|_{\rho=\bar{\rho}}$$

and

$$b_0 = B(\bar{\rho}) = D(\bar{\rho}) = d_0 \qquad [58]$$

If the entropy is a local functional of the density, $k(u,v)$ must be of the form $k(u,v) = f(\bar{\rho})\delta(u-v)$ which inserted in [57] gives

$$f(\bar{\rho}) = [\bar{\rho}(1-\bar{\rho})]^{-1} \qquad [59]$$

and

$$b_0[\bar{\rho}(1-\bar{\rho})]^{-1} - (d_1 - b_1) = 0 \qquad [60]$$

Therefore if b_0, b_1, d_1 do not satisfy the last equation, the entropy cannot be a local functional of the density. It can be shown that in this case time-reversal invariance is violated and the adjoint hydrodynamics is different from [50]. This calculation supports the conjecture that macroscopic correlations are a generic feature of equilibrium states of nonreversible lattice gases.

See also: Interacting Particle Systems and Hydrodynamic Equations; Interacting Stochastic Particle Systems; Nonequilibrium Statistical Mechanics (Stationary): Overview; Quantum Central-Limit Theorems.

Further Reading

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Magnetic Resonance Imaging

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Introduction

Nuclear magnetic resonance (NMR) is a subtle quantum-mechanical phenomenon that, through magnetic resonance imaging (MRI), has played a major role in the revolution in medical imaging over the last 30 years. Before being conceived for use in imaging, NMR was employed by chemists to do spectroscopy, and it remains a very important technique for determining the structure of complex chemical compounds like proteins. In this article we explain how NMR is used to create an image of a three-dimensional object. Scant attention is paid to both NMR spectroscopy, and the quantum description of NMR. Those seeking a more complete introduction to these subjects should consult the article Nuclear Magnetic Resonance in this Encyclopedia, as well as the monographs of Abragam (1983) or Ernst *et al.* (1987), for spectroscopy, and that of Callaghan (1993) for imaging. All three books consider the quantum-mechanical description of these phenomena. Comprehensive discussions of MRI can be found in Bernstein *et al.* (2004) and Haacke *et al.* (1999), and a historical appreciation of the development of MRI is given in Wehrli (1995).

The Bloch Equation

We begin with the Bloch phenomenological equation, which provides a model for the interactions between applied magnetic fields and the nuclear spins in the objects under consideration. This is a macroscopic averaged model that describes the interaction of aggregates of spins, called isochromats, with applied magnetic fields. An isochromat is a collection of "like" spins, which is spatially large on the atomic scale, but very small on the scale of the variations present in the applied magnetic fields. Spins are alike if they belong to the same species and are in the same chemical environment. There may be several different classes of spins, but, in this article, it is assumed that they are noninteracting and so it suffices to consider each separately. Heretofore, we suppose that there is a single class of like spins. The distribution of isochromats for these spins is described macroscopically by the spin density function, which we denote by $\rho(x,y,z)$. In most medical applications, one is imaging the distribution of spins arising from hydrogen protons in water molecules.

The state of the isochromat at spatial location (x,y,z) is given by a 3-vector:

$$\boldsymbol{M}(x,y,z) = (m_1(x,y,z), m_2(x,y,z), m_3(x,y,z))$$

which is interpreted as the magnetic moment per unit volume. It is an ensemble mean of the quantum dipoles caused by the spins within the isochromat. In most applications of NMR to imaging, the applied magnetic field is described as the sum of a large, time-independent field, $\boldsymbol{B}_0(x,y,z)$, and smaller time-dependent fields, $\boldsymbol{B}'(x,y,z;t)$. In the presence of a static field, thermal fluctuations cause the nuclear spins to slightly prefer an orientation aligned with the field. Using the Boltzmann distribution, one obtains that the nuclear paramagnetic susceptibility of water protons is given by

$$\chi = \frac{\hbar^2\gamma^2}{4k_B T} \qquad [1]$$

here $\hbar$ is Planck's constant, k_B the Boltzmann's constant, and T the absolute temperature, (see Levitt (2001)). The constant γ is called the gyromagnetic (or magnetogyric) ratio. For a proton,

$$\gamma \approx 2\pi \times 42.5764 \times 10^6 \text{ rad s}^{-1}\text{T}^{-1} \qquad [2]$$

For water molecules at room temperature, $\chi \approx 3.6 \times 10^{-9}$.

If the sample is held stationary in the field $\boldsymbol{B}_0$ for a sufficiently long time, then the spins become polarized and a bulk magnetic moment appears; this is called the equilibrium magnetization:

$$\boldsymbol{M}_0(x,y,z) = \chi\rho(x,y,z)\boldsymbol{B}_0(x,y,z) \qquad [3]$$

The Bloch equation describes the evolution of $\boldsymbol{M}$ under the influence of the applied field $\boldsymbol{B} = \boldsymbol{B}_0 + \boldsymbol{B}'$:

$$\frac{\mathrm{d}\boldsymbol{M}(x,y,z;t)}{\mathrm{d}t} = \gamma\boldsymbol{M}(x,y,z;t) \times \boldsymbol{B}(x,y,z;t) - \frac{1}{T_2}\boldsymbol{M}^{\perp}(x,y,z;t) + \frac{1}{T_1}(\boldsymbol{M}_0(x,y,z) - \boldsymbol{M}^{\parallel}(x,y,z;t)) \qquad [4]$$

Here $\times$ is the vector cross-product, $\boldsymbol{M}^{\perp}(x,y,z;t)$ the component of $\boldsymbol{M}(x,y,z;t)$ perpendicular to $\boldsymbol{B}_0(x,y,z)$ (called the transverse component), and $\boldsymbol{M}^{\parallel}$ the component of $\boldsymbol{M}$ parallel to $\boldsymbol{B}_0$ (called the longitudinal component). For hydrogen protons in other molecules, the gyromagnetic ratio is expressed in the form $(1-\sigma)\gamma$. The coefficient σ is called the

nuclear shielding; it is typically between -10^{-4} and $+10^{-4}$. The difference in the nuclear shielding causes a shift in the resonance frequency by $\gamma\sigma$.

The second and third terms in eqn [4] are relaxation terms. They provide a phenomenological model for the averaged interactions of the spins with one another and their environment. The coefficient $1/T_1(x, y, z)$ is the spin lattice relaxation rate; it describes the rate at which the magnetization returns to equilibrium. The coefficient $1/T_2(x, y, z)$ is the spin–spin relaxation rate; it describes the rate at which the transverse components of $\boldsymbol{M}$ decay. The physical processes causing these relaxation phenomena are different and so are the rates themselves, with T_2 less than T_1. The relaxation rates largely depend on the localized thermal fluctuations of the molecules and provide a useful contrast mechanism in MR imaging. Spin–spin relaxation occurs very rapidly in solids (<1 ms) and, therefore, we usually assume that we are imaging liquid-like materials such as water protons in soft mammalian tissues. In this case, T_2 takes values in the 40 ms to 4 s range. Notice that this model does not include any explicit interaction between isochromats at different spatial locations. A variety of such interactions exist, but, at least in liquid-like materials, they lead only to small corrections in the Bloch equation model. A derivation of the Bloch equation from the Schrödinger equation can be found in Abragam (1983) and Slichter (1990). For coupled systems, the Bloch equation formalism breaks down and a full quantum-mechanical treatment is necessary (*see* Nuclear Magnetic Resonance and Ernst *et al.* (1983)).

Much of the analysis in NMR imaging amounts to understanding the behavior of solutions to eqn [4] with different choices of $\boldsymbol{B}$. We now consider some important special cases. The simplest case occurs if $\boldsymbol{B}$ has no time-dependent component; then this equation predicts that the sample becomes polarized with the transverse part of $\boldsymbol{M}$ decaying as e^{-t/T_2}, and the longitudinal component approaching the equilibrium magnetization, $\boldsymbol{M}_0$, as $1 - e^{-t/T_1}$. To simplify the subsequent discussion, we assume that the field $\boldsymbol{B}_0$ is homogeneous with $\boldsymbol{B}_0 = (0, 0, b_0)$. If $\boldsymbol{B} = \boldsymbol{B}_0$ and we omit the relaxation terms (set $T_1 = T_2 = \infty$ in [4]), then an initial magnetization $\boldsymbol{M}(x, y, z; 0)$ simply precesses about $\boldsymbol{B}_0$ at angular frequency $\omega_0 = \gamma b_0 : \boldsymbol{M}(x, y, z; t) = U(t)\boldsymbol{M}(x, y, z; 0)$, with

$$U(t) = \begin{bmatrix} \cos\omega_0 t & -\sin\omega_0 t & 0 \\ \sin\omega_0 t & \cos\omega_0 t & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad [5]$$

The frequency ω_0 is called the Larmor frequency; this precession of $\boldsymbol{M}$ about the axis of $\boldsymbol{B}_0$ is the resonance phenomenon referred to as NMR. In typical medical imaging systems, b_0 is between 1 and 3 T and the corresponding resonance frequency is between 40 and 120 MHz.

Typically, the field $\boldsymbol{B}$ takes the form

$$\boldsymbol{B} = \boldsymbol{B}_0 + \tilde{\boldsymbol{G}} + \boldsymbol{B}_1 \qquad [6]$$

where $\tilde{\boldsymbol{G}}$ is a gradient field and $\boldsymbol{B}_1$ is a radio-frequency (RF) field. Usually, the gradient fields are "piecewise time-independent" fields, small relative to $\boldsymbol{B}_0$. By piecewise time-independent field, we mean a collection of static fields that, in the course of the experiment, are turned on and off. The $\boldsymbol{B}_1$ component is a time-dependent RF field, nominally at right angles to $\boldsymbol{B}_0$. It is usually taken to be spatially homogeneous, with time dependence of the form

$$\boldsymbol{B}_1(t) = U(t)\begin{pmatrix} \alpha(t) \\ \beta(t) \\ 0 \end{pmatrix} \qquad [7]$$

The functions α and β define an envelope that modulates the time-harmonic field, $[\cos\omega_0 t, \sin\omega_0 t, 0]$. They are supported in a finite interval $[t_0, t_1]$, that is, the $\boldsymbol{B}_1$ field is "turned on" for a finite period of time. The change in the state of the magnetization between t_0 and t_1 is called the RF excitation. It may be spatially dependent.

In light of [5] it is convenient to introduce the rotating reference frame. We replace $\boldsymbol{M}$ with $\boldsymbol{m}$, where $\boldsymbol{m}(x, y, z; t) = U(t)^{-1}\boldsymbol{M}(x, y, z; t)$. It is a classical result of Larmor, that if $\boldsymbol{M}$ satisfies [4], then $\boldsymbol{m}$ satisfies

$$\begin{aligned} \frac{d\boldsymbol{m}(x, y, z; t)}{dt} &= \gamma\boldsymbol{m}(x, y, z; t) \times \boldsymbol{B}_{\text{eff}}(x, y, z; t) \\ &\quad - \frac{1}{T_2}\boldsymbol{m}^{\perp}(x, y, z; t) + \frac{1}{T_1}(\boldsymbol{M}_0(x, y, z) \\ &\quad - \boldsymbol{m}^{\parallel}(x, y, z; t)) \end{aligned} \qquad [8]$$

where

$$\boldsymbol{B}_{\text{eff}} = U(t)^{-1}\boldsymbol{B} - \left(0, 0, \frac{\omega_0}{\gamma}\right)$$

As $\tilde{\boldsymbol{G}}$ is much smaller than $\boldsymbol{B}$ and quasistatic, it turns out that one can ignore the components of $\tilde{\boldsymbol{G}}$ orthogonal to $\boldsymbol{B}_0$. Indeed, in imaging applications, one usually assumes that the components of $\tilde{\boldsymbol{G}}$ depend linearly on (x, y, z) with the $\hat{z}$-component given by $\langle(x, y, z), (g_1, g_2, g_3)\rangle$. The constant vector $\boldsymbol{G} = (g_1, g_2, g_3)$ is called the gradient vector. With $\boldsymbol{B}_0 = (0, 0, b_0)$ and $\boldsymbol{B}_1$ given by [7], we see that $\boldsymbol{B}_{\text{eff}}$ can be taken to equal $(0, 0, \langle(x, y, z), \boldsymbol{G}\rangle) + (\alpha, \beta, 0)$.

In the remainder of this article, we assume that B_{eff} takes this form.

If $G = 0$ and $\beta \equiv 0$, then the solution operator for Bloch's equation, without relaxation terms, is

$$V(t) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta(t) & \sin\theta(t) \\ 0 & -\sin\theta(t) & \cos\theta(t) \end{bmatrix} \qquad [9]$$

where

$$\theta(t) = \int_0^t \alpha(s)\,\mathrm{d}s \qquad [10]$$

This is simply a rotation about the x-axis through the angle $\theta(t)$. If $B_1 \neq 0$ for $t \in [0, \tau]$, then the magnetization is rotated through the angle $\theta(\tau)$. Thus, RF excitation can be used to move the magnetization out of its equilibrium state. As we shall soon see, this is crucial for obtaining a measurable signal. Note that the equilibrium magnetization is a tiny perturbation of the very large field B_0 and is, therefore, in practice not directly measurable. Only the precessional motion of the transverse components of M produces a measurable signal. More general B_1 fields, that is, with both α and β nonzero, have more complicated effects on the magnetization. In general, the angle between M and M_0 at the conclusion of the RF excitation is called the flip angle.

If, on the other hand, $B_1 = 0$ and $G_l = (0, 0, l(x, y, z))$, where $l(\cdot)$ is a function, then V depends on (x, y, z), and is given by

$$V(x, y, z; t) = \begin{bmatrix} \cos\gamma l(x,y,z)t & -\sin\gamma l(x,y,z)t & 0 \\ \sin\gamma l(x,y,z)t & \cos\gamma l(x,y,z)t & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad [11]$$

This is precession about B_0 at an angular frequency that depends on the local field strength $b_0 + l(x, y, z)$. If both B_1 and $\tilde{G}$ are simultaneously nonzero, then, starting from equilibrium, the solution of the Bloch equation, at the conclusion of the RF pulse, has a nontrivial spatial dependence. In other words, the flip angle becomes a function of the spatial variables. We return to this in a later section.

A Basic Imaging Experiment

With these preliminaries, we can describe the basic measurements in magnetic resonance imaging. When exposed to B_0, the sample becomes polarized at a rate determined by T_1. Once the sample is polarized, a B_1-field, of the form given in [7] (with $\beta \equiv 0$), is turned on for a finite time τ. This is called an RF excitation. For the purposes of this discussion, we suppose that the time is chosen so that $\theta(\tau) = 90°$, see eqn [10]. As B_0 and B_1 are spatially homogeneous, the magnetization vectors within the object remain parallel throughout the RF excitation. At the conclusion of the RF excitation, M is orthogonal to B_0.

After the RF is turned off, the vector field $M(x, y, z; t)$ precesses about B_0, in phase with the angular velocity ω_0. The transverse component of M decays exponentially. If we normalize the time so that $t = 0$ corresponds to the conclusion of the RF pulse, then, in the laboratory frame,

$$M(x, y, z; t) = \frac{\chi\omega_0\rho(x, y, z)}{\gamma}\Big[\mathrm{e}^{-t/T_2}\cos\omega_0 t, \; \mathrm{e}^{-t/T_2}\sin\omega_0 t, (1 - \mathrm{e}^{-t/T_1})\Big] \qquad [12]$$

Recall Faraday's law: a changing magnetic field induces an electromotive force (EMF) in a loop of wire according to the relation

$$\mathrm{EMF}_{\text{loop}} \propto \frac{\mathrm{d}\Phi_{\text{loop}}}{\mathrm{d}t} \qquad [13]$$

Here Φ_{loop} denotes the flux of the field through the loop of wire (*see* Introductory Articles: Electromagnetism). The transverse components of M are a rapidly varying magnetic field, which, according to Faraday's law, induce a current in a loop of wire. In fact, by placing several such loops close to the sample we can measure a signal of the form

$$S_0(t) = \frac{\chi\omega_0^2 \mathrm{e}^{\mathrm{i}\omega_0 t}}{\gamma}\int_{\text{sample}} \rho(x, y, z)\mathrm{e}^{-t/T_2(x,y,z)} \times b_{1\text{rec}}(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \qquad [14]$$

Here $b_{1\text{rec}}(x, y, z)$ quantifies the sensitivity of the detector to the precessing magnetization located at (x, y, z). From $S_0(t)$ we easily obtain a measurement of the integral of the function $\rho b_{1\text{rec}}$. By using a carefully designed detector, $b_{1\text{rec}}$ can be taken to be a constant, and therefore we can determine the total spin density within the object of interest. For the rest of this article, we assume that $b_{1\text{rec}}$ is a constant. Note that the size of the measured signal is proportional to ω_0^2, which is, in turn, proportional to $\|B_0\|^2$. This explains, in part, why it is so useful to have a very strong B_0-field. Though even with a 1.5 T magnet, the measured signal is only in the microwatt range (see Hoult and Lauterbur (1979) and Edelstein *et al.* (2004)).

Suppose that, at the end of the RF excitation, we turn on the gradient $\tilde{G}$. As the magnetic field $B = B_0 + \tilde{G}$ now has a nontrivial spatial dependence, the precessional frequency of the spins, which equals

$\gamma\|\boldsymbol{B}\|$, also has a spatial dependence. In fact, assuming that T_2 is spatially independent, it follows from [11] that the measured signal would now be given by

$$S_G(t) \approx \frac{\chi b_{1\mathrm{rec}}\omega_0^2 \mathrm{e}^{-t/T_2}\mathrm{e}^{\mathrm{i}\omega_0 t}}{\gamma} \times \int_{\text{sample}} \rho(x,y,z)\mathrm{e}^{2\pi\mathrm{i}\langle(x,y,z),\boldsymbol{k}\rangle}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \qquad [15]$$

Up to a constant, $\mathrm{e}^{-\mathrm{i}\omega_0 t}\,\mathrm{e}^{-t/T_2}S_G(t)$ is simply the Fourier transform of ρ at $\boldsymbol{k} = -t\gamma\boldsymbol{G}/2\pi$. By sampling in time and using a variety of different gradient vectors, we can sample the three-dimensional Fourier transform of ρ in a neighborhood of 0. This suffices to reconstruct an approximation to ρ. In medical applications, T_2 is spatially dependent, which, as described later in the section "Contrast and resolution," provides a useful contrast mechanism.

Imagine that we collect samples of $\hat{\rho}(\boldsymbol{k})$ on a rectangular grid

$$\left\{(j_x\Delta k_x, j_y\Delta k_y, j_z\Delta k_z): -\frac{N_x}{2} \le j_x \le \frac{N_x}{2}, -\frac{N_y}{2} \le j_y \le \frac{N_y}{2}, -\frac{N_z}{2} \le j_z \le \frac{N_z}{2}\right\}$$

Since we are sampling in the Fourier domain, the Nyquist sampling theorem implies that the sample spacing determines the spatial field of view from which we can reconstruct an artifact-free image: in order to avoid aliasing artifacts, the support of ρ must lie in a rectangular region with side lengths $[\Delta k_x^{-1}, \Delta k_y^{-1}, \Delta k_z^{-1}]$, see Haacke *et al.* (1999), Epstein (2003), and Barrett and Myers (2004). In typical medical applications, the support of ρ is much larger in one dimension than the others, and so it turns out to be impractical to use the simple data collection technique described above. Instead, the RF excitation takes place in the presence of nontrivial gradient fields, which allows for a spatially selective excitation: the magnetization in one region of space obtains a transverse component, while that in the complementary region is left in the equilibrium state. In this way, we can collect data from an essentially two-dimensional slice. This is described in the next section.

Selective Excitation

As remarked above, practical imaging techniques do not excite all the spins in an object and directly measure samples of the three-dimensional Fourier transform. Rather, the spins lying in a slice are excited and samples of the two-dimensional Fourier transform are then measured. This process is called selective excitation and may be accomplished by applying the RF excitation with a gradient field turned on. With this arrangement, the strength of the static field, $\boldsymbol{B}_0 + \tilde{\boldsymbol{G}}$, varies with spatial position, hence the response to the RF excitation does as well. Suppose that $\tilde{\boldsymbol{G}} = (0, 0, \langle(x,y,z), \boldsymbol{G}\rangle)$ and set $f = [2\pi]^{-1}\gamma\langle(x,y,z), \boldsymbol{G}\rangle$. This is called the offset frequency, as it is the amount by which the local resonance frequency differs from the resonance frequency ω_0 of the $\boldsymbol{B}_0$-field. The result of a selective RF excitation is described by a magnetization profile $\boldsymbol{m}^{\mathrm{pr}}(f)$, which is a unit 3-vector-valued function of the offset frequency. A typical case would be

$$\boldsymbol{m}^{\mathrm{pr}}(f) = \begin{cases} [0, 0, 1] & \text{for } f \notin [f_0, f_1] \\ [\sin\theta, 0, \cos\theta] & \text{for } f \in [f_0, f_1] \end{cases} \qquad [16]$$

The magnetization is flipped through an angle θ, in regions of space where the offset frequency lies in the interval $[f_0, f_1]$ and is left in the equilibrium state otherwise.

Typically, the excitation step takes a few milliseconds and is much shorter than either T_1 or T_2; therefore, one generally uses the Bloch equation, without relaxation, in the discussion of selective excitation. In the rotating reference frame, the Bloch equation, without relaxation, takes the form

$$\frac{\mathrm{d}\boldsymbol{m}(f;t)}{\mathrm{d}t} = \begin{bmatrix} 0 & 2\pi f & -\gamma\beta \\ -2\pi f & 0 & \gamma\alpha \\ \gamma\beta & -\gamma\alpha & 0 \end{bmatrix} \boldsymbol{m}(f;t) \qquad [17]$$

The problem of designing a selective pulse is nonlinear. Indeed, the selective excitation problem can be rephrased as a classical inverse-scattering problem: one seeks a function $\alpha(t) + \mathrm{i}\beta(t)$ with support in an interval $[t_0, t_1]$ so that, if $\boldsymbol{m}(f;t)$ is the solution to (17) with $\boldsymbol{m}(f;t_0) = [0, 0, 1]$, then $\boldsymbol{m}(f;t_1) = \boldsymbol{m}^{\mathrm{pr}}(f)$. If one restricts attention to flip angles close to 0, then there is a simple linear model that can be used to find approximate solutions.

If the flip angle is close to zero, then $m_3 \approx 1$ throughout the excitation. Using this approximation, we derive the low-flip-angle approximation to the Bloch equation, without relaxation:

$$\frac{\mathrm{d}(m_1 + \mathrm{i}m_2)}{\mathrm{d}t} = -2\pi\mathrm{i}f(m_1 + \mathrm{i}m_2) + \mathrm{i}\gamma(\alpha + \mathrm{i}\beta) \qquad [18]$$

From this approximation, we see that

$$\alpha(t) + \mathrm{i}\beta(t) \approx \frac{\mathcal{F}(m_1^{\mathrm{pr}} + \mathrm{i}m_2^{\mathrm{pr}})(t)}{\gamma i} \quad \text{where } \mathcal{F}(h)(t) = \int_{-\infty}^{\infty} h(f)\mathrm{e}^{-2\pi i f t}\,\mathrm{d}f \qquad [19]$$

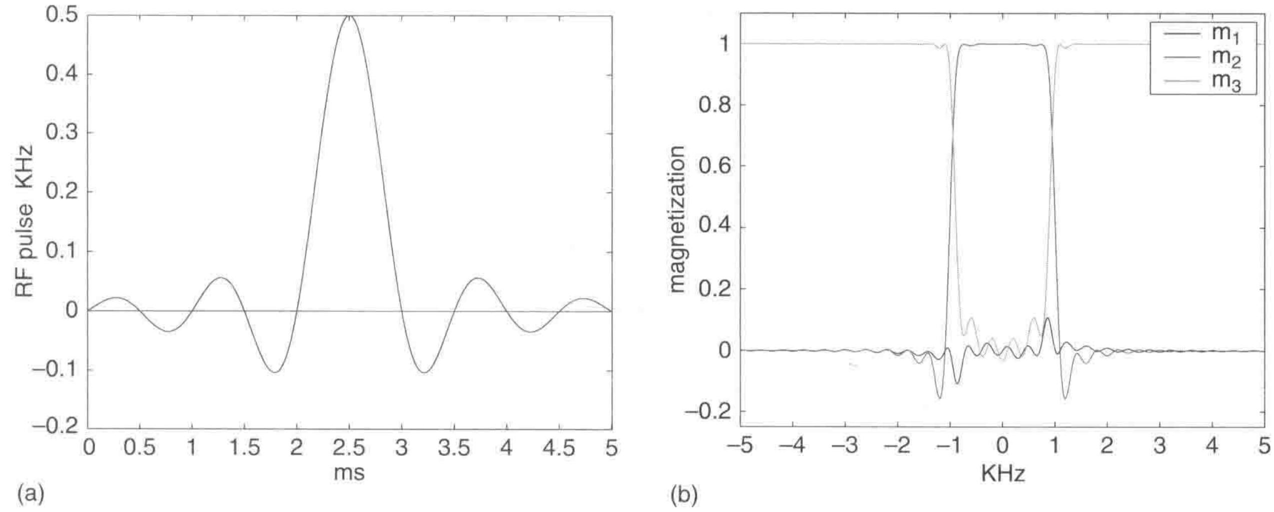


Figure 1 A selective 90° pulse and profile designed using the linear approximation. (a) Profile of a 90° sinc-pulse. (b) The magnetization profile produced by the pulse in (a).

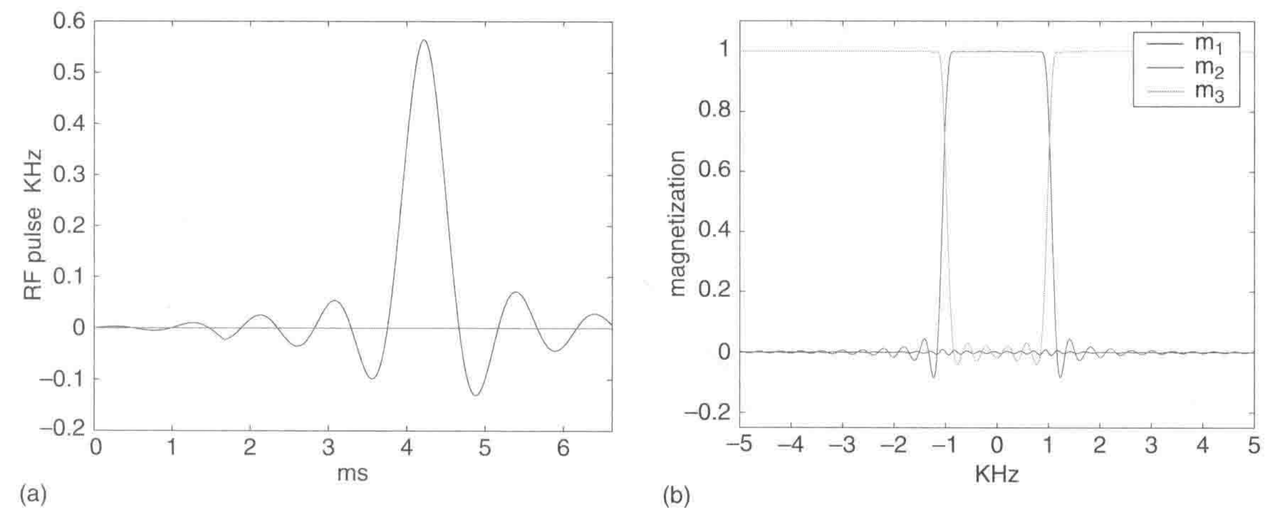


Figure 2 A selective 90° pulse and profile designed using the inverse scattering approach. (a) Profile of a 90° inverse-scattering pulse. (b) The magnetization profile produced by the pulse in (a).

For an example such as in [16], θ close to zero, and $f_0 = -f_1$, we obtain

$$\alpha + \mathrm{i}\beta \approx \frac{\mathrm{i}\sin\theta\sin f_1 t}{\pi\gamma t} \qquad [20]$$

A pulse of this sort is called a sinc-pulse. A sinc-pulse is shown in **Figure 1a**, the result of applying it in **Figure 1b**. A more accurate pulse can be designed using the Shinnar–Le Roux algorithm (see Pauly *et al.* (1991) and Shinnar and Leigh (1989)), or the inverse scattering approach (see Epstein (2004)). An inverse-scattering 90°-pulse is shown in **Figure 2a** and the response in **Figure 2b**.

Spin-Warp Imaging

In an earlier section we showed how NMR measurements could be used to measure the three-dimensional Fourier transform of ρ. In this section, we consider a more practical technique, that of measuring the two-dimensional Fourier transform of a "slice" of ρ. Applying a selective RF pulse, as described in the previous section, we can flip the magnetization in a region of space $z_0 - \Delta z < z < z_0 + \Delta z$, while leaving it in the equilibrium state outside a slightly larger region. Observing that a signal near the resonance frequency is only produced by isochromats whose magnetization has a nonzero transverse component, we can now measure samples of the two-dimensional Fourier transform of the function

$$\bar{\rho}_{z_0}(x, y) = \frac{1}{2\Delta z}\int_{z_0-\Delta z}^{z_0+\Delta z_0} \rho(x, y, z)\,\mathrm{d}z \qquad [21]$$

If Δz is sufficiently small then $\bar{\rho}_{z_0}(x, y) \approx \rho(x, y, z_0)$.

In order to be able to use the fast Fourier transform (FFT) algorithm to do the reconstruction, it is very useful to sample $\hat{\bar{\rho}}_{z_0}$ on a uniform grid. To that end, we use the gradient fields as follows: after the RF excitation we apply a gradient field of the form $\boldsymbol{G}_{\text{ph}} = (0, 0, -g_2 y + g_1 x)$ for a certain period of time T_{ph}. This is called a phase encoding gradient. At the conclusion of the phase encoding gradient, the transverse components of the magnetization from the excited spins has the form

$$\boldsymbol{m}^{\|}(x, y) \propto \mathrm{e}^{-2\pi \mathrm{i}(k_y y - k_x x)} \bar{\rho}_{z_0}(x, y) \qquad [22]$$

where $(k_x, k_y) = [2\pi]^{-1} \gamma T_{\text{ph}}(-g_1, g_2)$. At time T_{ph}, we turn off the y-component of $\boldsymbol{G}_{\text{ph}}$ and reverse the polarity of the x-component. At this point, we begin to measure the signal. We get samples of $\hat{\bar{\rho}}(k, k_y)$ where k varies from $-k_{x\max}$ to $k_{x\max}$. By repeating this process with the strength of the y-phase encoding gradient being stepped through a sequence of uniformly spaced values, $g_2 \in \{n\Delta g_y\}$, and collecting samples at a uniformly spaced set of times, we collect the set of samples

$$\left\{ \hat{\bar{\rho}}_{z_0}(m\Delta k_x, n\Delta k_y): -\frac{N_x}{2} \le m \le \frac{N_x}{2}, -\frac{N_y}{2} \le n \le \frac{N_y}{2} \right\} \qquad [23]$$

The gradient $\boldsymbol{G}_{\text{fr}} = (0, 0, -g_1 x)$, left "on" during signal acquisition, is called a frequency encoding gradient. While there is no difference, mathematically, between the phase encoding and frequency encoding steps, there are significant practical differences. This approach to sampling is known as spin-warp imaging; it was introduced in Edelstein *et al.* (1980). The steps of this experiment are summarized in a pulse sequence timing diagram, shown in **Figure 3**. This graphical representation for the steps followed in a magnetic resonance imaging experiment is ubiquitous in the literature.

To avoid aliasing artifacts, the sample spacings Δk_x and Δk_y must be chosen so that the excited portion of the sample is contained in a region of size $\Delta k_x^{-1} \times \Delta k_y^{-1}$. This is called the field of view or FOV. Since we can only collect the signal for a finite period of time, the Fourier transform $\hat{\bar{\rho}}(k_x, k_y)$ is sampled at frequencies lying in a rectangle with vertices $(\pm k_{x\max}, \pm k_{y\max})$, where

$$k_{x\max} = \frac{N_x \Delta k_x}{2}, \quad k_{y\max} = \frac{N_y \Delta k_y}{2} \qquad [24]$$

The maximum frequencies sampled effectively determine the resolution available in the reconstructed

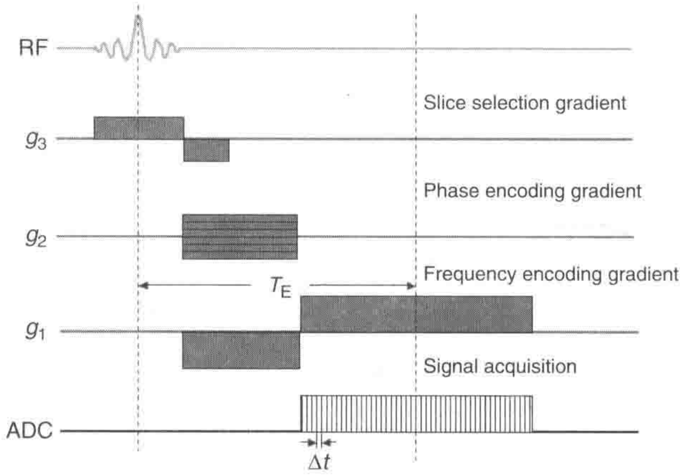


Figure 3 Pulse timing diagram for spin-warp imaging. During the positive lobe of the frequency encoding gradient, the analog-to-digital converter (ADC) collects samples of the signal produced by the rotating transverse magnetization.

image. Heuristically, this resolution limit equals half the shortest measured wavelength:

$$\begin{aligned} \Delta x &\approx \frac{1}{2k_{x\max}} = \frac{FOV_x}{N_x} \\ \Delta y &\approx \frac{1}{2k_{y\max}} = \frac{FOV_y}{N_y} \end{aligned} \qquad [25]$$

Whether one can actually resolve objects of this size in the reconstructed image depends on other factors such as the available contrast and the signal-to-noise ratio (SNR). We consider these factors in the final sections.

Signal-to-Noise Ratio

At a given spatial resolution, image quality is largely determined by SNR and the contrast between the different materials making up the imaging object. SNR in MRI is defined as the voxel signal amplitude divided by the noise standard deviation. The noise in the NMR signal, in general, is Gaussian distributed with zero mean. Ignoring contributions from quantization, for example, due to limitations of the analog-to-digital converter, the noise voltage of the signal can be ascribed to random thermal fluctuations in the receive circuit (see Edelstein (1986)). The variance is given by

$$\sigma^2_{\text{thermal}} = 4k_{\text{B}} TR\Delta\nu \qquad [26]$$

where k_{B} is Boltzmann's constant, T the absolute temperature, R the effective resistance (resulting from both receive coil, R_{c} and object, R_{o}), and $\Delta\nu$ the receive bandwidth. Both R_{c} and R_{o} are frequency dependent, with $R_{\text{c}} \propto \omega^{1/2}$, and $R_{\text{o}} \propto \omega$. Their relative contributions to overall circuit resistance depend in a complicated manner on coil geometry, and the imaging object's shape, size, and conductivity

(see Chen and Hoult (1989)). Hence, at high magnetic field, and for large objects, as in most medical applications, the resistance from the object dominates and the noise scales linearly with frequency. Since the signal is proportional to ω^2, in MRI, the SNR increases in proportion to the field strength.

As the reconstructed image is complex valued, it is customary to display the magnitude rather than the real component. This, however, has some consequences on the noise properties. In regions where the signal is much larger than the noise, the Gaussian approximation is valid. However, in regions where the signal is low, rectification causes the noise to assume a Raleigh distribution. Mean and standard deviation can be calculated from the joint probability distribution:

$$P(N_\mathrm{r}, N_\mathrm{i}) = \frac{1}{2\pi\sigma^2} \mathrm{e}^{-(N_\mathrm{r}^2 + N_\mathrm{i}^2)/2\sigma^2} \quad [27]$$

where N_r and N_i are the noise in the real and imaginary channels, respectively. When the signal is large compared to noise, one finds that the variance $\sigma_m^2 = \sigma^2$. In the other extreme of nearly zero signal, one obtains for the mean:

$$\widehat{S} = \sigma\sqrt{\pi/2} \cong 1.253\sigma \quad [28]$$

and, for the variance:

$$\sigma_m^2 = 2\sigma^2(1 - \pi/4) \cong 0.655\sigma^2 \quad [29]$$

Of particular practical significance is the SNR dependence on the imaging parameters. The voxel noise variance is reduced by the total number of samples collected during the data acquisition process, that is,

$$\sigma_m^2 = \sigma_\mathrm{thermal}^2 / N \quad [30]$$

where $N = N_x N_y$ in a two-dimensional spin-warp experiment. Incorporating the contributions to thermal noise variance, other than bandwidth, into a constant

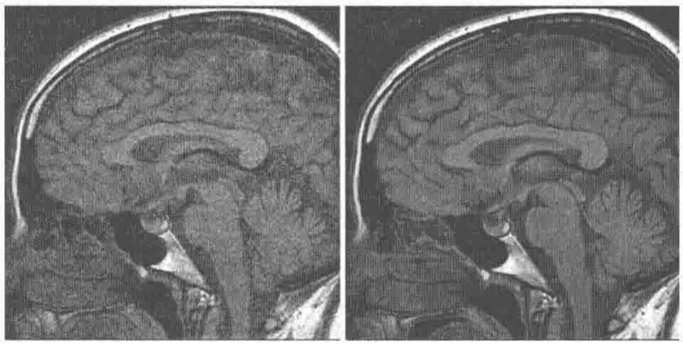
$$u = 4k_\mathrm{B}TR \quad [31]$$

we obtain for the noise variance:

$$\sigma_m^2 = \frac{u\Delta\nu}{N_x N_y N_\mathrm{avg}} \quad [32]$$

Here N_avg is the number of signal averages collected at each phase encoding step. We obtain a simple formula for SNR per voxel of volume ΔV:

$$\mathrm{SNR} = C\tilde{\rho}\,\Delta V \sqrt{\frac{N_x N_y N_\mathrm{avg}}{u\Delta\nu}} = C\tilde{\rho}\,\Delta x\,\Delta y\,d_z \sqrt{\frac{N_x N_y N_\mathrm{avg}}{u\Delta\nu}} \quad [33]$$



(a) (b)

Figure 4 T_1-weighted sagittal images through the midline of the brain: Image (b) has twice the SNR of image (a), showing improved conspicuity of small anatomic and low-contrast detail. The two images were acquired at 1.5 T field strength using two-dimensional spin-warp acquisition and identical scan parameters, except for N_avg, which was 1 in (a) and 4 in (b).

where $\Delta x, \Delta y$ are defined in [25], d_z is the thickness of the slab selected by the slice-selective RF pulse, and $\tilde{\rho}$ denotes the spin density weighted by effects determined by the (spatially varying) relaxation times T_1 and T_2 and the pulse sequence timing parameters. **Figure 4** shows two images of the human brain obtained from the same anatomic location but differing in SNR.

Contrast and Resolution

The single most distinctive feature of MRI is its extraordinarily large innate contrast. For two soft tissues, it can be on the order of several hundred percent. By comparison, contrast in X-ray imaging is a consequence of differences in the attenuation coefficients for two adjacent structures and is typically on the order of a few percent.

We have seen in the preceding sections that the physical principles underlying MRI are radically different from those of X-ray computed tomography, in that the signal elicited is generated by the spins themselves in response to an external perturbation. The contrast between two regions, A and B, with signals S_A and S_B, respectively, is defined as

$$C_{AB} = \frac{S_A - S_B}{S_A} \quad [34]$$

If the only contrast mechanism were differences in the proton spin density of various tissues, then contrast would be on the order of 5–20%. In reality, it can be several hundred percent. The reason for this discrepancy is that the MR signal is acquired under nonequilibrium conditions. At the time of excitation, the spins have typically not recovered from the effect of the previous cycle's RF pulses, nor

is the signal usually detected immediately after its creation.

Typically, in spin-warp imaging, a spin-echo is detected as a means to alleviate spin coherence losses from static field inhomogeneity. A spin-echo is the result of applying an RF pulse that has the effect of taking (m_1, m_2, m_3) to $(m_1, -m_2, -m_3)$. As such a pulse effects a 180° rotation of the $\hat{z}$-axis, it is also called a π-pulse. If, after such a pulse, the spins continue to evolve in the same environment then, following a certain period of time, the transverse components of the magnetization vectors throughout the sample become aligned. Hence a pulse of this type is also called a refocusing pulse. The time when all the transverse components are rephased is called the echo time, T_E.

The spin-echo signal amplitude for an RF pulse sequence $\pi/2 - \tau - \pi - \tau$, repeated every T_R seconds, is approximately given by

$$S(t = 2\tau) \approx \rho(1 - e^{-T_R/T_1})e^{-T_E/T_2} \qquad [35]$$

This is a good approximation as long as $T_E << T_R$ and $T_2 << T_R$, in which case the transverse magnetization decays essentially to zero between successive pulse sequence cycles. In eqn [35], ρ is voxel spin density and the echo time $T_E = 2\tau$. Empirically, it is known that tissues differ in at least one of the intrinsic quantities, T_1, T_2, or ρ. It, therefore, suffices to acquire images in such a manner that contrast is sensitive to one particular parameter. For example, a "T_2-weighted" image would be acquired with $T_E \sim T_2$ and $T_R >> T_1$ and, similarly, a "T_1-weighted" image with $T_R < T_1$ and $T_E << T_2$, with T_1, T_2 representing typical tissue proton relaxation times. **Figure 5** shows two images obtained with the same scan parameters except for T_R and T_E illustrating the fundamentally different image contrasts that are achievable.

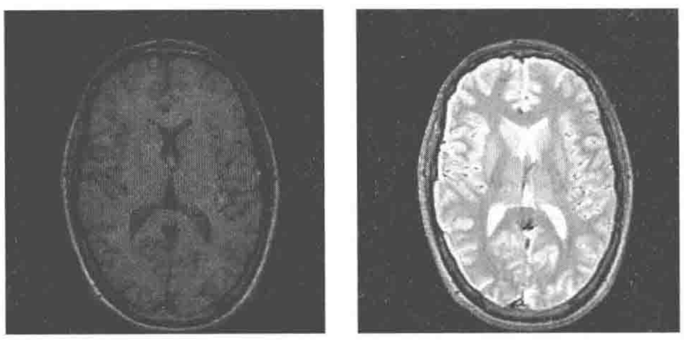
It is noteworthy that object visibility is not just determined by the contrast between adjacent structures but is also a function of the noise. It is, therefore, useful to define the contrast-to-noise ratio as

$$\mathrm{CNR}_{AB} = \frac{C_{AB}}{\sigma_{\mathrm{eff}}} \qquad [36]$$

where σ_{eff} is the effective standard deviation of the signal. Finally, it may be useful to reconstruct parametric images in which the pixel signal values represent any one of the intrinsic parameters. A T_2-image can be computed from eqn [35], for example, either analytically from two image data sets acquired with two different echo times, or from a series of T_E values, obtained from a Carr–Purcell spin-echo train, using regression techniques (*see* Nuclear Magnetic Resonance and Haacke *et al.* (1999)).

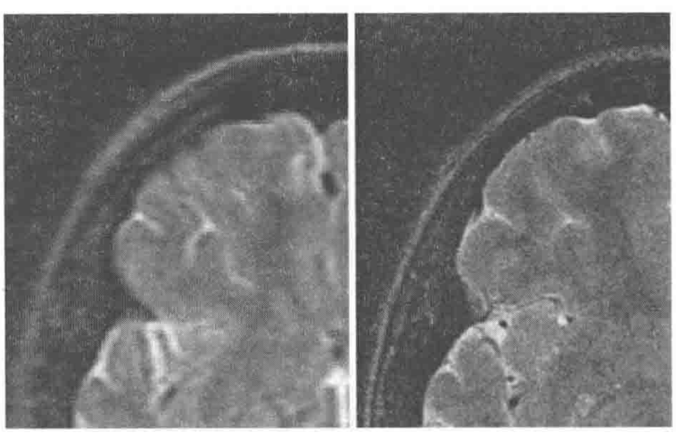
We have previously shown that the limiting resolution is given by $k_{\max}$, the largest spatial frequency sampled, see [25]. In reality, however, the actual resolution is always lower. For example, spin–spin (T_2) relaxation causes the signal to decay during the acquisition. In spin-warp imaging, this causes the high spatial frequencies to be further attenuated.

A further consequence of finite sampling is a ringing or Gibbs artifact that is most prominent at sharp intensity discontinuities. In practice, these artifacts are mitigated by applying an appropriate apodizing filter to the data. **Figure 6** shows a portion of a brain image obtained at two different resolutions. In **Figure 6b**, the total ***k***-space area covered was 16 times larger than for the acquisition of the image in a). Artifacts from finite sampling and blurring of fine detail such as cortical blood vessels are clearly visible in the low-resolution image. SNR, according to eqn [33], is reduced in the latter image by a factor of 4.



(a) (b)

Figure 5 Dependence of image contrast on pulse sequence timing parameters: (a) T_1-weighted; (b) proton density-weighted.



(a) (b)

Figure 6 Effect of ***k***-space coverage on spatial resolution in axial image of the brain: the field of view in both images was 20 cm and all scan parameters were the same except that (a) was acquired with $N_x = N_y = 128$ and (b) with $N_x = N_y = 512$.

See also: Nuclear Magnetic Resonance; Stochastic Resonance.

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Magnetohydrodynamics

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The Basic Modeling

Magnetohydrodynamics (MHD) is the study of the interaction of (electro-) magnetic fields and conducting fluids. When a conducting fluid (e.g., a liquid metal, a weakly ionized gas, or a plasma) is placed within a magnetic field, two coupling phenomena appear: the electric currents modify the magnetic field, and the Lorentz forces due to the magnetic field modify the motion of the fluid. At the mathematical level, two sets of equations, very different in nature, are involved. The usual description of the hydrodynamics phenomena is most often that provided by the continuum mechanics for fluids, while the description of electromagnetic phenomena essentially proceeds from the Maxwell equations.

Either category of equations can be declined in a variety of models. The coupling between the two categories might also be accounted for at different levels of accuracy. For the sake of conciseness in such an expository survey, it is neither desirable nor doable to present all the possible set of equations and their possible coupling. The difficulty stems from the incredibly large spectrum of physical phenomena where MHD plays a role. A list of such phenomena includes

- astrophysical and geophysical applications (modeling of stars in the galactic field, of pulsars, of solar spots, of the flows in the earth's core, ...),
- advanced "terrestrial" applications such as the magnetic confinement of plasmas in controlled fusion, MHD propulsion engines for rockets, and
- industrial applications in the engineering world (electromagnetic pumping, metal forming, aluminum electrolysis, and many other metallurgical applications).

Due to this variety of physical situations, no unified setting can be presented with a satisfactory degree of details. We therefore mostly concentrate throughout this article on the MHD of conducting fluids that are homogeneous, incompressible, viscous, and Newtonian. This is often the case of liquid metals in many industrial processes. The equations manipulated will first be given in their most general form and then immediately adapted to the above context. For other contexts, the modeling follows the same pattern, but other variants of the general equations must be employed. The bibliography of this article contains such general information.

The Hydrodynamics Description

The usual description for fluids follows from continuum mechanics. In this setting, the governing equation is the equation for the conservation of momentum

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \operatorname{div}(\rho \boldsymbol{u} \otimes \boldsymbol{u}) - \operatorname{div}\tau = f \qquad [1]$$

where ρ denotes the density of the fluid, $\boldsymbol{u}$ its velocity, τ the stress tensor, and f the density of volumic (or per unit volume) body forces applied to the fluid. For incompressible viscous Newtonian fluids, the stress/velocity relation reads

$$\tau = \eta(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\mathrm{T}}) - p\mathrm{Id} \qquad [2]$$

together with the constraint

$$\operatorname{div} \boldsymbol{u} = 0 \qquad [3]$$

on the velocity. Here, η denotes the viscosity of the fluid, p the pressure, and A^{T} denotes the transpose matrix of the matrix A. A third usual assumption is that the incompressible fluid is in addition homogeneous, that is,

$$\rho = \bar{\rho} = \text{constant} \qquad [4]$$

Equations [1]–[4] lead to the equations for conservation of momentum in the case of incompressible homogeneous viscous Newtonian fluid, that is, the incompressible Navier–Stokes equations

$$\begin{aligned} \bar{\rho}\frac{\partial \boldsymbol{u}}{\partial t} + \bar{\rho}\boldsymbol{u} \cdot \nabla \boldsymbol{u} - \eta \Delta \boldsymbol{u} + \nabla p &= f \\ \operatorname{div} \boldsymbol{u} &= 0 \end{aligned} \qquad [5]$$

These equations are supplied with initial and boundary conditions on the velocity $\boldsymbol{u}$. At initial time, the velocity is assumed to be known $\boldsymbol{u}(t=0,\cdot) = \boldsymbol{u}_0$ on the whole domain occupied by the fluid Ω, a domain that is supposed here not to vary in time (see, nevertheless, the section "The industrial production of aluminum" for a different setting). On the other hand, the boundary conditions on the boundary $\partial\Omega$ of Ω can be of various forms. For simplicity, the boundary is supposed regular, so that its unitary outward normal $\boldsymbol{n}_{\partial\Omega}$ can be unambiguously defined. The standard choice is to set Dirichlet conditions on the velocity $\boldsymbol{u} = \boldsymbol{u}_{\text{given}}$. In the following, we will assume for simplicity that the boundary condition is the homogeneous Dirichlet boundary condition $\boldsymbol{u} = 0$, as a superposition of the nonpenetration condition $\boldsymbol{u} \cdot \boldsymbol{n}_{\partial\Omega} = 0$ and the no-slip boundary condition $\boldsymbol{u} \times \boldsymbol{n}_{\partial\Omega} = 0$. One can also impose alternative boundary conditions, for example, involving the pressure.

The Electromagnetic Description

Classical electromagnetism is described by the Maxwell equations. For the sake of consistency, we recall here that these are:

The Maxwell–Ampère equation

$$-\frac{\partial \boldsymbol{D}}{\partial t} + \operatorname{curl} \boldsymbol{H} = \boldsymbol{j} \qquad [6]$$

The Maxwell–Coulomb equation

$$\operatorname{div} \boldsymbol{D} = \rho_{\mathrm{c}} \qquad [7]$$

The Maxwell–Faraday equation

$$\frac{\partial \boldsymbol{B}}{\partial t} + \operatorname{curl} \boldsymbol{E} = 0 \qquad [8]$$

The Maxwell–Gauss equation

$$\operatorname{div} \boldsymbol{B} = 0 \qquad [9]$$

In the above equations, the three-dimensional vector fields $\boldsymbol{D}$, $\boldsymbol{B}$, $\boldsymbol{E}$, $\boldsymbol{H}$ denote the electric and magnetic inductions, and the electric and magnetic fields, respectively. On the other hand, the three-dimensional vector field $\boldsymbol{j}$ denotes the current density, and the scalar field ρ_{c} denotes the charge density. Inside an electrically conducting medium, the standard assumption of perfect medium consists in assuming the following relations:

$$\begin{aligned} \boldsymbol{D} &= \varepsilon \boldsymbol{E} \\ \boldsymbol{H} &= \frac{1}{\mu}\boldsymbol{B} \end{aligned} \qquad [10]$$

often called "constitutive laws," where ε and μ, respectively, denote the (electric) permittivity and the (magnetic) permeability of the medium. In the simple isotropic homogeneous case, both these parameters are scalar and constant. They are often expressed as

$$\begin{aligned} \varepsilon &= \varepsilon_{\mathrm{r}}\varepsilon_0 \\ \mu &= \mu_{\mathrm{r}}\mu_0 \end{aligned} \qquad [11]$$

where ε_0, μ_0 are the permittivity and the permeability of the vaccum (that satisfy $\varepsilon_0\mu_0 = 1/c^2$, with c denoting the speed of light), and ε_{r}, μ_{r} are the permittivity and the permeability relative to vaccum, or relative permittivity and relative permeability.

When collecting [6]–[9], together with [10], [11], one obtains the following general system of

Maxwell equations in a continuum (dielectric) medium:

$$
\begin{aligned}
-\frac{\partial(\varepsilon E)}{\partial t} + \operatorname{curl}\left(\frac{1}{\mu}B\right) &= j \\
\operatorname{div}(\varepsilon E) &= \rho_c \\
\frac{\partial B}{\partial t} + \operatorname{curl} E &= 0 \\
\operatorname{div} B &= 0
\end{aligned}
\qquad [12]
$$

This system is supplied with initial conditions on the fields B and E. On the other hand, boundary conditions might be necessary when the equations are restricted to a bounded domain. The latter question, quite delicate, is postponed until next section.

The MHD Coupling

For coupling systems [5] and [12], a threefold task is in order.

On the one hand, the body force term in [5] needs to be made precise, and this is completed by setting

$$f = j \times B + f_{\text{ext}} \qquad [13]$$

The first term in the right-hand side is the Lorentz force, consequence of the electric current j running within the magnetic field B, a force that influences the motion, along the velocity field u, of the particles of the conducting fluid. The second term is due to possible external forces. A typical case for such forces is that of the gravity forces

$$f_{\text{ext}} = \bar{\rho} g \qquad [14]$$

On the other hand, in order to be a mathematically closed system, the Maxwell system [12] needs to be complemented by Ohm's law, another type of constitutive relation, like [10], that now relates the current density j with the other fields. When dealing with MHD phenomena, Ohm's law most often reads in the form

$$j = \sigma(E + u \times B) \qquad [15]$$

where σ denotes the electric conductivity of the fluid. The second term of [15] explicitly accounts for the deviation of the lines of electric current by the hydrodynamics flow. In some oversimplified situations, it can be neglected, leading to Ohm's law in the more usual form $j = \sigma E$, that is also valid for solid media. Most of the times the term $u \times B$ contains crucial information, and thus is not neglected.

System [5]–[12] now reads

$$
\begin{aligned}
\bar{\rho}\frac{\partial u}{\partial t} + \bar{\rho} u \cdot \nabla u - \eta \Delta u + \nabla p &= j \times B + f_{\text{ext}} \\
\operatorname{div} u &= 0 \\
-\frac{\partial(\varepsilon E)}{\partial t} + \operatorname{curl}\left(\frac{1}{\mu}B\right) &= j \\
\operatorname{div} E &= \frac{1}{\varepsilon}\rho_c \\
\frac{\partial B}{\partial t} + \operatorname{curl} E &= 0 \\
\operatorname{div} B &= 0 \\
j &= \sigma(E + u \times B)
\end{aligned}
\qquad [16]
$$

A third task is then in order.

Apart from the constitutive laws [10] and Ohm's law [15], the specificity of the Maxwell equations for conducting fluids, as opposed to the same equations written, for example, in the vacuum, resides in the possible need for supplying the system with *ad hoc* boundary conditions. Indeed, in their most general form, the Maxwell equations are valid in the whole physical space $\mathbb{R}^3$. On the other hand, as the goal here is to simulate an MHD fluid that most often occupies only a bounded domain Ω in $\mathbb{R}^3$, there is the need to adequately define the simulation domain.

A first possibility is to set the Maxwell equations in the whole space, while solving the hydrodynamics equation on the domain Ω occupied by the fluid. Regarding only the Maxwell equations [12], this seems to be the method of choice. But then there is the need for an extension of Ohm's law [15] outside the fluid domain. Notice indeed that u appears in [15]. In addition to this, the fact that the physical confinement device for the fluid is then embedded in the domain where the Maxwell equations are set may be the source of various difficulties, as such a device is often delicate to model and treat. Therefore, alternative tracks may be followed.

A second possibility is to restrict the Maxwell equation to a bounded domain. In turn, this option divides in two: taking as the domain for the Maxwell equations that occupied by the fluid, or choosing a domain larger than Ω. We cannot discuss this choice without loss of generality, and refer the reader to the literature (see e.g., Gerbeau *et al.* (2005)). In either situation, boundary conditions are needed. We only consider the former for the sake of brevity.

A standard choice for the boundary conditions for [12] is the following:

$$
\begin{aligned}
E \times n_{\partial\Omega} &= k \times n_{\partial\Omega} \\
B \cdot n_{\partial\Omega} &= q
\end{aligned}
\qquad [17]
$$

where $\boldsymbol{k}$ and q, respectively, are given vector and scalar functions on the boundary.

A fact that needs to be emphasized is that it is not so easy to design accurate boundary conditions, that is, evaluations of $\boldsymbol{k}$ or g, especially because accurate experimental measures of magnetic quantities are often delicate to obtain, especially in industrial environments.

A Commonly Used Simplified MHD Coupling

For the terrestrial MHD applications that are the focus of the present article, a commonly used assumption is to neglect the first term $\partial(\varepsilon E)/\partial t$, often called the displacement current, in the Maxwell–Ampère equation [6], that is the first equation of [12] or the third of [16] above. Then system [16] can be reorganized, eliminating $\boldsymbol{E}$ and $\boldsymbol{j}$, and leaving aside the Maxwell–Faraday equation [8], Ohm's law [15], and the Maxwell–Coulomb equation [7]. The latter equations amount to defining, respectively, $\boldsymbol{E}$ from $\boldsymbol{B}, \boldsymbol{j}$ from $\boldsymbol{E}$ and $\boldsymbol{B}$, and ρ_c from $\boldsymbol{E}$. One is left with the following system with the triple of unknown fields $(\boldsymbol{u}, p, \boldsymbol{B})$

$$\begin{gathered}\bar{\rho}\frac{\partial \boldsymbol{u}}{\partial t} + \bar{\rho}\boldsymbol{u}\cdot\nabla\boldsymbol{u} - \eta\Delta\boldsymbol{u} + \nabla p = \frac{1}{\mu}\operatorname{curl}\boldsymbol{B}\times\boldsymbol{B} + \boldsymbol{f}_{\text{ext}} \\ \operatorname{div}\boldsymbol{u} = 0 \\ \frac{\partial \boldsymbol{B}}{\partial t} + \operatorname{curl}\left(\frac{1}{\sigma}\operatorname{curl}\frac{1}{\mu}\boldsymbol{B}\right) = \operatorname{curl}(\boldsymbol{u}\times\boldsymbol{B}) \\ \operatorname{div}\boldsymbol{B} = 0\end{gathered} \qquad [18]$$

Correspondingly, the initial conditions are now only on the pair $(\boldsymbol{u}, \boldsymbol{B})$. Regarding the boundary conditions on $\boldsymbol{B}$, they can be derived from [17] using, for example, a homogeneous Dirichlet boundary condition on $\boldsymbol{u}$:

$$\begin{gathered}\operatorname{curl}\boldsymbol{B}\times\boldsymbol{n}_{\partial\Omega} = \tilde{\boldsymbol{k}}\times\boldsymbol{n}_{\partial\Omega} \\ \boldsymbol{B}\cdot\boldsymbol{n}_{\partial\Omega} = q\end{gathered} \qquad [19]$$

Other simplifications of system [16] can be adopted, such as steady-state approximations. In particular, it is often considered that electromagnetic phenomena have characteristic times that are so short in comparison with the characteristic time of hydrodynamics phenomena that the Maxwell equations in their stationary form may be coupled to the time-dependent hydrodynamics equations, such as [5]. We refer to the "Further reading" section for further information along these lines (see e.g., Gerbeau *et al.* (2005)).

The Mathematical Nature of the Equations

With a view to understand the mathematical nature of systems [16] and [18], we first briefly recall some mathematical facts concerning hydrodynamics, before focusing on the coupling with electromagnetics.

Regarding the incompressible Navier–Stokes equation, we recall that the state of the art of the mathematical knowledge heavily depends on the dimension of the ambient space. In dimension 2, solutions are unique and regular (they are said to be strong), for regular enough data of course. Unfortunately, as the focus is here on MHD and electromagnetism is fundamentally a three-dimensional phenomenon, only the three-dimensional case for the Navier–Stokes equation is relevant. Now, in the context of the Navier–Stokes equations alone, only the existence of weak solutions for large times, and the existence and uniqueness of strong solutions for small times are known. Whether or not there exists a unique strong solution for all time (of course again for sufficiently regular data) is an open problem, of outstanding difficulty, (see Temam 1995).

In the coupled setting examined here, there is no reason to expect a better situation. At best, one may hope for the same situation as that for the uncoupled case (Navier–Stokes equations alone). Regarding the existence and uniqueness of solutions, a commonly used strategy is that of regularization: the Cauchy problem is studied for regularized data, and then one passes to the limit in the regularization. In this latter step, the linear terms cause no difficulty, since they pass to the limit only using weak convergence. On the other hand, the main concern is always the treatment of the nonlinear terms, which require strong convergence. Here, for the Navier–Stokes equation in the MHD setting, the additional difficulty stems from the presence of the nonlinear term $\boldsymbol{j}\times\boldsymbol{B}$ on the right-hand side. The mathematical treatment of this nonlinear term calls for a compactness argument, which in turn requires obtaining some information on the fields $\boldsymbol{j}$ and $\boldsymbol{B}$, and their derivatives, from the Maxwell equations. In this respect, the situation is radically different for system [16] and for system [18]. Likewise, these two systems behave differently regarding the other nonlinear term of electromagnetic nature, namely $\boldsymbol{u}\times\boldsymbol{B}$ in Ohm's law, or $\operatorname{curl}(\boldsymbol{u}\times\boldsymbol{B})$ on the right-hand side of the equation in $\boldsymbol{B}$, respectively.

The Hyperbolic Variant

Due to the presence of the Maxwell equations [12] in their general form, that is a hyperbolic form,

system [16] is indeed very difficult, from the standpoint of mathematical analysis.

In order to realize this, it suffices to recall that the first step in the proof of the existence of solution to such a system of equations is to write down an *a priori* energy estimate. It is a simple manipulation on [16] to show that, formally, a solution to [16] satisfies

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \overline{\rho}|\boldsymbol{u}|^2 + \eta\int_\Omega |\nabla \boldsymbol{u}|^2 = \int_\Omega (\boldsymbol{j}\times\boldsymbol{B})\cdot\boldsymbol{u} \qquad [20]$$

multiplying the Navier–Stokes equation by $\boldsymbol{u}$ and integrating over the domain Ω, while, on the other hand,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \varepsilon|\boldsymbol{E}|^2 + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{\mu}|\boldsymbol{B}|^2 = -\int_\Omega \boldsymbol{j}\cdot\boldsymbol{E} \qquad [21]$$

multiplying the Maxwell–Ampère equation by $-\boldsymbol{E}$, the Maxwell–Faraday equation by $(1/\mu)\boldsymbol{B}$, integrating over Ω, and summing up the two. Next, the right-hand side of [21] can be modified, accounting for Ohm's law:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \varepsilon|\boldsymbol{E}|^2 + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{\mu}|\boldsymbol{B}|^2 = -\int_\Omega \frac{1}{\sigma}|\boldsymbol{j}|^2 - \int_\Omega (\boldsymbol{j}\times\boldsymbol{B})\cdot\boldsymbol{u} \qquad [22]$$

Summing up [20] and [22] yields the energy estimate:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(\overline{\rho}|\boldsymbol{u}|^2 + \varepsilon|\boldsymbol{E}|^2 + \frac{1}{\mu}|\boldsymbol{B}|^2\right) + \int_\Omega \frac{1}{\sigma}|\boldsymbol{j}|^2 + \eta\int_\Omega |\nabla\boldsymbol{u}|^2 = 0 \qquad [23]$$

Notice that, in the above, we set the external forces and all boundary conditions to zero, for the sake of simplicity.

Estimate [23] clearly indicates that we dispose of $L^\infty([0,T],L^2(\Omega))$ bounds on the vector fields $\boldsymbol{E}$ and $\boldsymbol{B}$ together with an $L^2([0,T]\times\Omega)$ bound on the current $\boldsymbol{j}$, and with the (classical) $L^\infty([0,T], L^2(\Omega))\cap L^2([0,T],H^1(\Omega))$ bounds on the velocity $\boldsymbol{u}$. In addition, $\operatorname{div}\boldsymbol{B}$ and, when assuming ρ_c bounded, $\operatorname{div}\boldsymbol{E}$ are bounded in $L^\infty([0,T]\times\Omega)$. Unfortunately, these bounds do not allow for passing to the limit in the nonlinear term $\boldsymbol{j}\times\boldsymbol{B}$ on the right-hand side of the Navier–Stokes equation. In addition, there seems to be no way of deriving further energy estimates on system [16] that would provide with more *a priori* regularity on the fields $\boldsymbol{E},\boldsymbol{B}$, and $\boldsymbol{j}$. To date, system [16] presents an unsolved mathematical difficulty.

The Parabolic Variant

On the other hand, system [18] is radically different in mathematical nature, because the Maxwell equations then reduce to a parabolic-type equation. The same manipulations as above, in order to establish *a priori* estimates on the solution of [18], now lead to

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(\overline{\rho}|\boldsymbol{u}|^2 + \frac{1}{\mu}|\boldsymbol{B}|^2\right) + \int_\Omega \frac{1}{\sigma}\left|\operatorname{curl}\left(\frac{1}{\mu}\boldsymbol{B}\right)\right|^2 + \eta\int_\Omega |\nabla\boldsymbol{u}|^2 = 0 \qquad [24]$$

which, together with the divergence-free constraint on $\boldsymbol{B}$, yields $L^\infty([0,T],L^2(\Omega))\cap L^2([0,T],H^1(\Omega))$ bounds on both the velocity $\boldsymbol{u}$ and the magnetic field $\boldsymbol{B}$. These bounds now allow for passing to the limit in the terms $\operatorname{curl}\boldsymbol{B}\times\boldsymbol{B}$ and $\operatorname{curl}(\boldsymbol{u}\times\boldsymbol{B})$ on the right-hand side of the equations. This being established, the rest of the mathematical analysis is straightforward, and a theorem of existence and uniqueness of solutions can be proved. Like in the case of the Navier–Stokes equations alone, we have (in dimension 3) the existence of a global-in-time weak solution (i.e., for any $T,\boldsymbol{u}$ and $\boldsymbol{B}$ both $L^\infty([0,T],L^2(\Omega))\cap L^2([0,T],H^1(\Omega))$ satisfying the divergence-free constraint). No uniqueness of this weak solution is known. On the other hand, for sufficiently regular data, we have the existence of a local-in-time strong solution (i.e., for T sufficiently small, $\boldsymbol{u}$ and $\boldsymbol{B}$ both $L^\infty([0,T],H^1(\Omega))\cap L^2([0,T], H^2(\Omega))$, and uniqueness of this strong solution in the class of weak solutions as long as it exists. We refer to Sermange and Temam, (1983) and Gerbeau *et al.* (2005).

At this stage, it is to be remarked that there is a formal similarity, at first sight at least, between the parabolic form of the Maxwell equations, namely

$$\begin{gathered}\frac{\partial\boldsymbol{B}}{\partial t} + \operatorname{curl}\operatorname{curl}\boldsymbol{B} = \operatorname{curl}\boldsymbol{h}\\ \operatorname{div}\boldsymbol{B} = 0\end{gathered} \qquad [25]$$

and the incompressible Navier–Stokes equation [5]. Note that indeed the curl operator in the first equation of [25] can be replaced by (minus) the Laplacian operator $-\Delta$, since $\operatorname{div}\boldsymbol{B}=0$. Actually, this formal similarity cannot be translated into mathematical arguments, simply because there is no pressure in [25]. In other terms, the divergence-free constraint $\operatorname{div}\boldsymbol{B}=0$ simply propagates in time in [25] (note that the right-hand side $\operatorname{curl}\boldsymbol{h}$ is also

divergence-free by construction), while on the other hand $\operatorname{div} \boldsymbol{u} = 0$ is enforced as a constraint in [5], the pressure playing the role of a Lagrange multiplier that adjusts itself in time in order to allow for $\boldsymbol{u}$ to be divergence-free.

Of course, as in the purely hydrodynamics case, much more can be said on the equations than simply establishing the existence and uniqueness of solutions. For instance, the long time limit of the solutions can be studied, etc.... For this and other issues, we refer to the "Further reading" section (Duvaut and Lions 1972a, b, Sermange and Temam 1983, Gerbeau *et al.* 2005).

Numerical Issues

We concentrate again on system [18]. It is illustrative to mention that this system, when written in nondimensional variables, reads

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \nabla \boldsymbol{u} - \frac{1}{Re} \Delta \boldsymbol{u} + \nabla p = S \operatorname{curl} \boldsymbol{B} \times \boldsymbol{B} + \boldsymbol{f}_{\text{ext}}$$

$$\operatorname{div} \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{B}}{\partial t} + \frac{1}{Re_{\text{mag}}} \operatorname{curl}(\operatorname{curl} \boldsymbol{B}) = \operatorname{curl}(\boldsymbol{u} \times \boldsymbol{B})$$

$$\operatorname{div} \boldsymbol{B} = 0$$

where S is the coupling parameter, Re is the (hydrodynamic) Reynolds number, and Re_{mag} denotes the magnetic Reynolds number.

As expected, the numerical simulation of a system such as [18] superposes the difficulties of the hydrodynamics simulation of incompressible viscous fluids, and those faced when simulating the parabolic form of the Maxwell equations. Therefore, the goal is to efficiently combine the techniques employed to overcome either of them.

For incompressible fluid mechanics, the method of choice is the finite-element method for the discretization of differential operators in space. A typical discretization of eqn [5], called the "mixed" finite-element method, makes use of a pair of finite elements, one for the velocity, and one for the pressure. Other possibilities exist, that amount more or less in eliminating one unknown in a first stage and calculating the second one as a postprocessing task. The mixed formulation in the pair of unknowns $(\boldsymbol{u}, p)$ is however the most employed method to date, at least in the present setting. The finite-element space for the velocity is taken richer than that for the pressure: a possibility is, for example, to take the degree of the finite element for the velocity equal to the degree of the finite element for the pressure plus one. The heuristics for this is the fact that the velocity is derived twice in [5] while the pressure is only derived once. Of course, a mathematical ground for this is available, and a key issue is the "inf–sup" condition (also compatibility condition, or stability condition) that dictates the possible choice for finite-elements pairs, so that problem [5] is well posed at the discrete level. Typically, $Q2$ finite elements for the velocity can be combined with (continuous) $Q1$ finite elements for the pressure. An alternative choice is to ignore the inf–sup condition, adopting, for example, $Q1$ finite elements for both fields $\boldsymbol{u}$ and p, but this requires for a so-called stabilized formulation of [5] at the discrete level. The "Further reading" section provides details on the broad variety of techniques available in the field: Quarteroni and Valli (1997), Gerbeau *et al.* (2005).

On the other hand, the parabolic equation on $\boldsymbol{B}$ in [18] may be discretized with the same finite elements as those used for the velocity. The enforcement of the divergence constraint $\operatorname{div} \boldsymbol{B} = 0$ at the discrete level deserves some attention. Recall indeed that at the continuous level the divergence-free constraint is spontaneously propagated by the equation. At the discrete level, a crucial role in this respect is played by the weak formulation of the parabolic equation and an *ad hoc* account for the boundary condition [17].

For the sake of completeness, let us mention that an alternative strategy to the use of the finite elements that have been mentioned above (and that are called Lagrangian finite elements), is to use "edge elements." In some sense, the use of such elements simplifies the treatment of the boundary conditions [17], since they are very well adapted to their mathematical nature.

Note also that, in the vein of what is done for purely hydrodynamics flow simulations, stabilized finite-elements techniques have been developed for the MHD system [18], that allow for a discretization of the three unknown fields $(\boldsymbol{u}, p, \boldsymbol{B})$ over the same finite elements, for example, $Q1$.

When coupling the two discrete formulations for simulating the whole system [18], two main strategies can be adopted: one can either treat each of the two equations separately, independently describing the propagation of $\boldsymbol{u}$ and $\boldsymbol{B}$ forward in time, or one can address directly the coupled system of equations, describing the propagation of $\boldsymbol{u}$ and $\boldsymbol{B}$ in parallel.

The first option aims in particular at obtaining in the end small algebraic systems. An instance of such

a segregated algorithm reads, formally and setting all constants to unity for simplicity,

$$\begin{aligned} &\frac{u^{n+1}-u^n}{\Delta t}+u^n\cdot\nabla u^{n+1}-\Delta u^{n+1}+\nabla p^{n+1} \\ &\quad=\operatorname{curl}B^n\times B^n+f_{\text{ext}} \\ &\operatorname{div}\,u^{n+1}=0 \\ &\frac{B^{n+1}-B^n}{\Delta t}+\operatorname{curl}\operatorname{curl}B^{n+1} \\ &\quad=\operatorname{curl}(u^n\times B^{n+1}) \\ &\quad\operatorname{div}B^{n+1}=0 \end{aligned} \qquad [26]$$

At each time step, the two independent subsystems are solved, providing with u^{n+1} and B^{n+1} for the next time step. The difficulty is that it is not possible, with such segregated algorithms, to reproduce the energy estimate [24] at the discrete level. Note that, at the continuous level, the estimate [24] is based upon a proper cancelation of the term $\int_\Omega (j\times B)\cdot u$ present on the two right-hand sides. Such a cancelation basically stems for a nonlinear interplay that cannot be present in a segregated iteration. Consequently, some spurious energy is created in the system simply by an inadequate iteration between the two equations. More precisely, the scheme obtained is at best only conditionally stable, that is, stable for small enough time steps, a condition that might be prohibitive when it is needed to simulate the MHD coupling over large times.

On the other hand, the other option consists in attacking the full system [18] directly:

$$\begin{aligned} &\frac{u^{n+1}-u^n}{\Delta t}+u^n\cdot\nabla u^{n+1}-\Delta u^{n+1}+\nabla p^{n+1} \\ &\quad=\operatorname{curl}\,B^{n+1}\times B^n+f_{\text{ext}} \\ &\operatorname{div}\,u^{n+1}=0 \\ &\frac{B^{n+1}-B^n}{\Delta t}+\operatorname{curl}\operatorname{curl}B^{n+1} \\ &\quad=\operatorname{curl}(u^{n+1}\times B^n) \\ &\quad\operatorname{div}\,B^{n+1}=0 \end{aligned} \qquad [27]$$

Note that B^{n+1} is present in the equation yielding u^{n+1}, while conversely u^{n+1} is present in that yielding B^{n+1}. Then the coupled system admits at the discrete level an energy estimate analogous to the energy estimate [24], and the scheme is much more stable than the previous one, and even unconditionally stable. The price to pay is that the system is, at the algebraic level, of very large size. Being sparse, it may however be treated, for example, via a GMRES-type iterative solver.

Let us make a final remark on these numerical issues. In the whole generality, the numerical simulation of viscous fluids raises the question of large Reynolds numbers, that is, the question of the difficulties encountered in the numerical approximation for viscosities η small with respect to the other dimensionalized parameters of the problem (density, velocity, and dimension of the domain). For such small viscosities, the flow becomes turbulent rather than laminar, and the broad range of length and energy scales in the flow turns out to be too difficult to capture numerically. A commonly used technique that is resorted to in such difficult cases is the turbulence modeling. Schematically, an averaged, or homogenized, model is derived on the basis of the Navier–Stokes equation, with the help of simplifying hypotheses, for example, in the form of closure relations. The quality of the simulation of the averaged model, and its relation to the true flow, heavily depends on these simplifying assumptions, which are in turn based upon a very deep understanding on the various physical phenomena at play. In the context of MHD flows, the situation is not clear, regarding such assumptions. It seems that there are no well-established models for turbulent MHD to date, at least from a rigorous viewpoint. In the absence of those, only a direct simulation of the Navier–Stokes equation seems possible.

The Industrial Production of Aluminium

A prototypical example of an application of MHD to the industrial context is the production of aluminum in electrolysis cells. The numerical simulation of the process involves the simulation of the evolution of two layers of nonmiscible incompressible viscous fluids, separated by an interface, and covered by a free surface. A schematic description of an industrial cell indeed is the following. An electric current of 10^5 A, or more, runs through two horizontal layers of conducting fluids: a bath of aluminum oxide above, and a layer of liquid aluminum below. The aluminum is produced by the reduction of the aluminum oxide, a reaction that only occurs at a temperature where aluminum is liquid. The high magnetic field induced by such a huge current produces in turn high Lorentz forces that influence the motion of either fluid. A key issue in the modeling, as well as in the technological control of the cell, is to understand the motion of the interface separating the two fluids. In a rough picture, this interface may be seen as a mobile

cathode, moving below a fixed anode. The equations describing the interior of the cell are basically of the type [18], with an important modification though: one needs to account for the presence of two fluids. They read:

$$\begin{aligned}\frac{\partial(\rho\boldsymbol{u})}{\partial t} &+ \operatorname{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u}) - \operatorname{div}(\eta(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)) \\ &= -\nabla p + \rho\boldsymbol{g} + \frac{1}{\mu}\operatorname{curl}\boldsymbol{B}\times\boldsymbol{B} \\ &\operatorname{div}\boldsymbol{u} = 0 \\ &\frac{\partial\rho}{\partial t} + \operatorname{div}(\rho\boldsymbol{u}) = 0 \\ \frac{\partial\boldsymbol{B}}{\partial t} &+ \operatorname{curl}\left(\frac{1}{\mu\sigma}\operatorname{curl}\boldsymbol{B}\right) = \operatorname{curl}(\boldsymbol{u}\times\boldsymbol{B}) \\ &\operatorname{div}\boldsymbol{B} = 0\end{aligned} \qquad [28]$$

where $\boldsymbol{g}$ denotes the gravity field, we recall, and are supplied with the boundary conditions

$$\begin{aligned}\boldsymbol{u} &= 0 \\ \frac{1}{\mu\sigma}\operatorname{curl}\boldsymbol{B}\times\boldsymbol{n}_{\partial\Omega} &= \boldsymbol{k}\times\boldsymbol{n}_{\partial\Omega} \\ \boldsymbol{B}.\boldsymbol{n}_{\partial\Omega} &= q\end{aligned} \qquad [29]$$

As opposed to [18], the density ρ in [28] is no longer the constant $\bar{\rho}$, but is only piecewise constant, that is, constant in each (moving) subdomain occupied by each fluid. Likewise, the viscosity η, and the conductivity σ are taken constant in each fluid, but with different values from one fluid to the other. While the density and the viscosity are only slightly different, the conductivity varies from many orders of magnitude, a discrepancy which ends up in some numerical stiffness of the equations. On the other hand, the permeability μ can be considered as constant throughout the domain, within a good level of approximation.

Mathematically, system [28] is an order of magnitude more difficult than [18]. We refer to Lions (1996) and Gerbeau and LeBris (1997) for some mathematical ingredients. A first major difficulty stems from the fact that the domain occupied by the fluids is no longer fixed. Notice that this difficulty already arises when simulating the MHD of one conducting fluid with a free surface. A second major difficulty is the discontinuity of the physical parameters at the interface, which causes a loss of regularity at the interface for the solution fields. The best result known to date is the existence of a global-in-time weak solution to [28]. Both mathematical difficulties above of course have significant numerical counterparts. A notable issue in such a simulation is how to handle the motion of the free interface, while ensuring that each fluid remains of constant mass (or volume) throughout the simulation. One of the most efficient method in such a context, introduced three decades ago, is the arbitrary-Lagrangian Eulerian (ALE) method. We refer to Brackbill and Pracht (1973) and Gerbeau *et al.* (2003a, b, 2005).

Apart from the direct numerical attack of system [28], which carries significant analytical and geometrical nonlinearities, there is the possibility, in particular in the industrial context, to derive a set of linearized equations at the vicinity of some equilibrium configuration of the system. This track has been extensively followed in the past and provides information that efficiently complement those provided by the much more satisfactory, but also more costly, nonlinear approach.

See also: Compressible Flows: Mathematical Theory; Computational Methods in General Relativity: The Theory; Fluid Mechanics: Numerical Methods; Newtonian Fluids and Thermohydraulics; Partial Differential Equations: Some Examples; Stability of Flows; Symmetric Hyperbolic Systems and Shock Waves; Topological Knot Theory and Macroscopic Physics.

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Malliavin Calculus

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Introduction

Malliavin calculus was initiated in 1976 with the work by P Malliavin (1978) and is essentially an infinite-dimensional differential calculus on the Wiener space. Its initial goal was to give conditions ensuring that the law of a random variable has a density with respect to Lebesgue measure as well as estimates for this density and its derivatives. When the random variables are solutions of stochastic differential equations (SDEs), these densities are heat kernels and Malliavin used Hörmander-type assumptions on the corresponding operators, thus providing a probabilistic proof of a Hörmander-type theorem for hypoelliptic operators.

The theory was much developed in the 1980s by Stroock, Bismut, and Watanabe, among others (the reader is referred to Nualart (1995) and Malliavin (1997)). In recent years, Malliavin calculus had great success in probabilistic numerical methods, mainly in the field of stochastic finance (Malliavin and Thalmaier 2005). However, the theory has also been applied to other fields of mathematics and physics, notably in statistical mechanics and statistical hydrodynamics (*see* Stochastic Hydrodynamics). In addition, one should remember that Wiener measure can be viewed as an "imaginary time" (but well-defined) counterpart of Feynman's "measure" for quantum systems. A stochastic calculus of variations for Wiener functionals could not be irrelevant to the path-integral approach to quantum theory.

Another field of application worth mentioning is the study of representations of stochastic oscillatory integrals with quadratic phase function and their stationary phase estimation. For this, complexification of the Wiener space must be properly defined (Malliavin and Taniguchi (1997)).

In order to give a flavor of what Malliavin calculus is all about, let us consider a second-order differential operator in $\mathbb{R}^d$ of the form

$$\mathcal{A} = \frac{1}{2}\sum_{i,j=1} a^{ij}\partial^2_{i,j} + \sum_i b^i\partial_i$$

with smooth bounded coefficients and such that the matrix a is symmetric and non-negative, admitting a square root σ. The corresponding Cauchy value problem consists in finding a smooth solution $u(t,x)$ of

$$\frac{\partial u}{\partial t} = \mathcal{A}u, \quad u(0,.) = \phi(.) \qquad [1]$$

Then there exists a transition probability function $p(t,x,.)$ such that

$$u(t,x) = \int_{\mathbb{R}^d} \phi(y)p(t,x,\mathrm{d}y)$$

When $p(t,x,\mathrm{d}y) = p(t,x,y)\mathrm{d}y$, the function p is the heat kernel associated to the operator $\mathcal{A}$, and from eqn [1] one may deduce Focker–Planck's equation for p.

Since Kolmogorov we know that it is possible to associate with such a second-order operator a stochastic family of curves like a deterministic flow is associated with a vector field. This stochastic family is a Markov process, $\xi_x(t)$, which is adapted to the increasing family $\mathcal{P}_\tau, \tau \in [0,1]$, of sigma-fields generated by the past events, that is, $u(\tau) \in \mathcal{P}_\tau$ for every τ.

Itô calculus allows us to write the SDE satisfied by ξ:

$$\mathrm{d}\xi(t) = \sigma(\xi_x(t))\,\mathrm{d}W(t) + b(\xi_x(t))\,\mathrm{d}t, \quad \xi_x(0) = x \qquad [2]$$

where $W(t)$ stands for $\mathbb{R}^d$-valued Brownian motion (*see* Stochastic Differential Equations). Then p is the image of the Wiener measure μ (the law of Brownian motion), namely $p(t,x,.) = \mu \circ \xi_x^{-1}(t)(.)$ and we have the representation

$$u(t,x) = E_\mu(\phi(\xi_x(t)))$$

The following criterion for absolute continuity of measures in finite dimensions holds:

Lemma *If γ is a probability measure on $\mathbb{R}^d$ and, for every $f \in C_b^\infty$,*

$$\left| \int \partial_i f \, \mathrm{d}\gamma \right| \leq c_i \|f\|_\infty$$

where c_i, $i = 1, \ldots, d$, are constants, then γ is absolutely continuous with respect to Lebesgue measure.

Now one can think about Wiener measure as an infinite (actually continuous) product of finite-dimensional Gaussian measures. Considering the toy model of the above-mentionned situation in one dimension, we replace Wiener measure by $\mathrm{d}\gamma(x) = (1/\sqrt{2\pi})\mathrm{e}^{-x^2/2}\,\mathrm{d}x$ and look at the process at a fixed time as a function g on $\mathbb{R}$. In order to apply the lemma and study the law of g, one would write

$$\int (f' \circ g)\,\mathrm{d}\gamma = \int \frac{(f \circ g)'}{g'}\,\mathrm{d}\gamma$$

and then integrate by parts to obtain $\int (f \circ g)\rho\,\mathrm{d}\gamma$. A simple computation shows that $\rho(x) = (g'' + xg')/(g')^2$, and, in particular, that the nondegeneracy of the derivative of g plays a role in the existence of the density.

To work with functionals on the Wiener space, one needs an infinite-dimensional calculus. Of course, other (Gateaux, Fréchet) calculi on infinite-dimensional settings are already available but the typical functionals we are dealing with, solutions of SDEs, are not continuous with respect to the underlying topology, nor even defined at every point, but only almost everywhere. Malliavin calculus, as a Sobolev differential calculus, requires very little regularity, given that there is no Sobolev imbedding theory in infinite dimensions.

Differential Calculus on the Wiener Space

We restrict ourselves to the classical Wiener space, although the theory may be developed in abstract Wiener spaces, in the sense of Gross. For a description of this theory as well as of Segal's model developed in the 1950s for the needs of quantum field theory, the reader is referred to Malliavin (1997).

Let $\mathcal{H}$ be the Cameron–Martin space, $\mathcal{H} = \{h : [0,1] \to \mathbb{R}^d$ such that $\dot{h}$ is square integrable and $h(t) = \int_0^t \dot{h}(\tau)\mathrm{d}\tau\}$, which is a separable Hilbert space with scalar product $<h_1, h_2> = \int_0^1 \dot{h}_1(\tau).\dot{h}_2(\tau)\mathrm{d}\tau$. The classical Wiener measure will be denoted by μ; it is realized on the Banach space X of continuous paths on the time interval [0,1] starting from zero at time zero, a space where $\mathcal{H}$ is densely imbedded. In finite dimensions, Lebesgue measure can be characterized by its invariance under the group of translations. In infinite dimensions there is no Lebesgue measure and this invariance must be replaced by quasi-invariance for translations of Wiener measures (Cameron–Martin admissible shifts). We recall that, if $h \in \mathcal{H}$, Cameron–Martin theorem states that

$$E_\mu(F(\omega + h)) = E_\mu\left(F(\omega)\exp\left(\int_0^1 \dot{h}(\tau)\,\mathrm{d}\omega(\tau) - \frac{1}{2}\int_0^1 |\dot{h}(\tau)|^2\,\mathrm{d}\tau\right)\right)$$

where $\mathrm{d}\omega$ denotes Itô integration.

For a cylindrical "test" functional $F(\omega) = f(\omega(\tau_1), \ldots, \omega(\tau_m))$, where $f \in C_b^\infty(\mathbb{R}^m)$ and $0 \leq \tau_1 \leq \cdots \leq \tau_m \leq 1$, the derivative operator is defined by

$$D_\tau F(\omega) = \sum_{k=1}^m \mathbf{1}_{\tau < \tau_k} \partial_k f(\omega(\tau_1), \ldots, \omega(\tau_m)) \qquad [3]$$

This operator is closed in $W_{2,1}(X; \mathbb{R})$, the completion of the space of cylindrical functionals with respect to the Sobolev norm

$$||F||_{2,1} = E_\mu ||F||^2 + E_\mu \int_0^1 |D_\tau F|^2\,\mathrm{d}\tau$$

Define F to be $\mathcal{H}$-differentiable at $\omega \in X$ when there exists a linear operator $\nabla F(\omega)$ such that, for all $h \in \mathcal{H}$,

$$F(\omega + h) - F(\omega) = \langle \nabla F(\omega), h \rangle + o(||h||_H) \quad \text{as } ||h|| \to 0$$

Then D_τ disintegrates the derivative in the sense that

$$D_h F(\omega) \equiv \langle \nabla F(\omega), h \rangle = \int_0^1 D_\tau F(\omega).\dot{h}(\tau)\,\mathrm{d}\tau \qquad [4]$$

Higher (r)-order derivatives, as r-linear functionals, can be considered as well in suitable Sobolev spaces.

Denote by δ the L^2_μ adjoint of the operator ∇, that is, for a process $u : X \to \mathcal{H}$ in the domain of δ, the divergence $\delta(u)$ is characterized by

$$E_\mu(F\delta(u)) = E_\mu\left(\int_0^1 D_\tau F.\dot{u}(\tau)\,\mathrm{d}\tau\right) \qquad [5]$$

For an elementary process u of the form $u(\tau) = \sum_j F_j(\tau \wedge \tau_j)$, where the F_j are smooth random variables and the sum is finite, the divergence is

$$\delta(u) = \sum_j F_j \omega(\tau_j) - \sum_j \int_0^{\tau_j} D_\tau F_j\,\mathrm{d}\tau$$

The characterization of the domain of δ is delicate, since both terms in this last expression are not independently closable. It can be shown that $W_{1,2}(X;H)$ is in the domain of δ and that the following "energy" identity holds:

$$E_\mu(\delta(u))^2 = E_\mu\|u\|_H^2 + E_\mu \int_0^1 \int_0^1 D_\tau \dot{u}_\sigma . D_\sigma \dot{u}_\tau \, d\sigma \, d\tau$$

Notice that when u is adapted to $\mathcal{P}_\tau$, Cameron–Martin–Girsanov theorem implies that the divergence coincides with Itô stochastic integral $\int_0^1 \dot{u}(\tau)\, d\omega(\tau)$ and, in this adapted case, the last term of the energy identity vanishes. We recover the well-known Itô isometry which is at the foundation of the construction of this integral. When the process is not adapted, the divergence turns out to coincide with a generalization of Itô integral, first defined by Skorohod.

The relation [5] is an integration-by-parts formula with respect to the Wiener measure μ, one of the basic ingredients of Malliavin calculus. This formula is easily generalized when the base measure is absolutely continuous with respect to μ.

Considering all functionals of the form $\mathcal{P}(\omega) = Q(\omega(\tau_1), \ldots, \omega(\tau_m))$ with Q a polynomial on $\mathbb{R}^d$, the Wiener chaos of order n, $\mathcal{C}_n$, is defined as $\mathcal{C}_n = \mathcal{P}_n \bigotimes \mathcal{P}_{n-1}^\perp$, where $\mathcal{P}_n$ denote the polynomials on X of degree $\leq n$. The Wiener-chaos decomposition $L_\mu^2(X) = \bigoplus_{n=0}^\infty \mathcal{C}_n$ holds. Denoting by Π_n the orthogonal projection onto the chaos of order n, we have

$$\left\langle \nabla\left(\prod_{n+1} F\right), h \right\rangle = \prod_n (\langle \nabla F, h\rangle)$$

The derivative D_u corresponds to the annihilation operator $A(u)$ and the divergence $\delta(u)$ to the creation operator $A^+(u)$ on bosonic Fock spaces.

An important result, known as the Clark–Bismut–Ocone formula, states that any functional $F \in W_{1,2}(X;\mathbb{R})$ can be represented as

$$F = E_\mu(F) + \int_0^1 E_\tau(D_\tau F)\, d\omega(\tau)$$

where E_τ denotes the conditional expectation with respect to the events prior to time τ (or, for short, the past $\mathcal{P}_\tau$ of τ).

The Ornstein–Uhlenbeck generator (or minus number operator) is defined by $\mathcal{L}F = -\delta\nabla F$. On cylindrical functionals $F(\omega) = f(\omega(\tau_1), \ldots, \omega(\tau_m))$, it has the form

$$\mathcal{L}F(\omega) = \sum_{i,j} \sigma_i \wedge \sigma_j \partial_{i,j}^2 f(\omega(\tau_1), \ldots, \omega(\tau_m)) - \sum_j \omega(\tau_j)\partial_j f(\omega(\tau_1), \ldots, \omega(\tau_m))$$

where i,j denote multi-dimensional (d) indexes.

As a multiplicative operator on the Wiener-chaos decomposition $\mathcal{L}F = -\sum_n n\Pi_n F$. It is the generator of a positive μ-self-adjoint semigroup, the Ornstein–Uhlenbeck semigroup, formally given by $T_t F = \sum_n e^{-nt}\Pi_n F$. Another familiar representation of this semigroup is Mehler formula,

$$T_t F(\omega) = E_\mu\left(F\left(e^{-t}\omega + \sqrt{(1 - e^{-2t}} v\right) d\mu(v) \right)$$

Considering the map $X \to \mathbb{R}^m, \omega \to (\omega(\tau_1), \ldots, \omega(\tau_m))$, the image of this operator is the Ornstein–Uhlenbeck generator (corresponding to the Langevin equation) on $\mathbb{R}^m$ with Euclidean metric defined by the matrix $\tau_i \wedge \tau_j$.

The fundamental theorem concerning existence of the density laws of Wiener functionals is the following:

Theorem *Let F be an $\mathbb{R}^d$-valued Wiener functional such that F^i and $\mathcal{L}F^i$ belong to L_μ^4 for every $i = 1, \ldots, d$. If the covariance matrix*

$$\langle \nabla F^i, \nabla F^j \rangle_{\mathcal{H}}$$

is almost surely invertible, then the law of F is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^d$.

Under more regularity assumptions, smoothness of the density is also derived. On the other hand, the integrability assumptions on $\mathcal{L}$ can be replaced by integrability of the second derivatives, due to Krée–Meyer inequalities on the Wiener space.

We remark that, although equivalent, the initial formulation (Malliavin 1978) of Malliavin calculus was different, relying on the construction of the two-parameter process associated to $\mathcal{L}$ and on its properties. In the early 1980s, the theory was elaborated, the main applications being the study of heat kernels (cf., e.g., Stroock (1981), Ikeda and Watanabe (1989), and Bismut (1984)). Starting from an SDE [2], it is possible to apply these techniques to obtain existence and smoothness of the transition probability function $p(t, x, y)$ if the vector fields $Z_i = \sum_j \sigma^{ij}(\partial/\partial x_j)$ together with their Lie brackets generate the tangent space for "sufficientely many" (in terms of probability) paths. These results shed a new light on Hörmander theorem for partial differential equations.

Quasi-Sure Analysis

Quasi-sure analysis is a refinement of classical probability theory and, generally speaking, replaces the fact that, due to Sobolev imbedding theorems, functions in finite dimensions belonging to Sobolev

classes are in fact smooth. We work in classical probability up to sets of probability zero; in quasi-sure analysis negligible sets are smaller and are those of capacity zero. This is the class of sets which are not charged by any measure of finite energy.

Under a nondegenerate map, Wiener measure and more general Gaussian measures may be disintegrated through a co-area formula. This principle, developed by Malliavin and co-authors (cf. Malliavin (1997) and references therein), implies that a property which is true quasi-surely will also hold true almost surely under conditioning by such a map. One can use this principle to study finer properties of SDEs. It was also used in M P Malliavin and P Malliavin (1990) to transfer properties from path to loop groups (*see* Measure on Loop Spaces). A pinned Brownian motion, for example, is well defined in quasi-sure analysis. It is possible to treat anticipative problems using quasi-sure analysis by solving the adapted problem after restriction of the solution to the finite-codimensional manifold which describes the anticipativity. These methods have also been applied to the computation of Lyapunov exponents of stochastic dynamical systems (Imkeller 1998). With a geometry of finite-codimensional manifolds of Wiener spaces well established, it is reasonable to think about applications to cases where such submanifolds correspond to level surfaces of invariant quantities for infinite-dimensional dynamical systems (cf. Cipriano (1999) for an example of such a situation in hydrodynamics).

The (p,r)-capacity of an open subset O of the Wiener space is defined by

$$\mathrm{cap}_{p,r}(O) = \inf\{\|\phi\|^p_{W_{2r}}, \phi \geq 0, \phi \geq 1\ \mu\text{-a.s. on } O\}$$

and, for a general set B, $\mathrm{cap}_{p,r}(B) = \inf\{\mathrm{cap}_{p,r}(O): B \subset O, O \text{ open}\}$. A set is said to be slim if all its (p,r)-capacities are zero. For $\Phi \in W_\infty$, the space of functionals with every Malliavin derivative belonging to all L^p_μ, there exists a redefinition of Φ, denoted by Φ^*, which is smooth and defined on the complement of a slim set.

Following Airault and Malliavin (1988), let $G \in W_\infty(X;\mathbb{R}^d)$ be of maximal rank and nondegenerate in the sense that the inverse of

$$(\det\Phi)^2(\omega) = \det(\langle\nabla\Phi^i(\omega), \nabla\Phi^j(\omega)\rangle)$$

belongs to W_∞. Then for every functional $G \in W_\infty$, the measures $\mu\circ\Phi^{-1}$ and $(G\mu)\circ\Phi^{-1}$ are absolutely continuous with respect to Lebesgue measure on $\mathbb{R}^d$ and have C^∞ Radon–Nikodym derivatives. If

$$\rho(\lambda) = \frac{\mathrm{d}\mu\circ\Phi^{-1}}{\mathrm{d}\lambda} \quad \text{and} \quad \rho_G(\lambda) = \frac{\mathrm{d}(G\mu)\circ\Phi^{-1}}{\mathrm{d}\lambda}$$

the function $\lambda \to \rho_G(\lambda)/\rho(\lambda)$ will be smooth in the open set $\mathcal{O} = \{\lambda : \rho(\lambda) > 0\}$.

For every $\lambda \in \mathcal{O}$, it is possible to define (up to slim sets) a submanifold of the Wiener space of codimension d, $\mathcal{S}_\lambda = (\Phi^*)^{-1}(\lambda)$, as well as a measure μ_S satisfying

$$\int_{\mathcal{S}_\lambda} G^*\,\mathrm{d}\mu_S(\omega) = E^{\Phi(\omega)=\lambda}(G) = \frac{\rho_G(\lambda)}{\rho(\lambda)}$$

for every $G \in W_\infty$. This measure does not charge slim sets.

The area measure $\aleph$ on the submanifold $\mathcal{S}_\lambda$ is defined by

$$\int F^*\,\mathrm{d}\aleph = \rho(\lambda)\int F^*(\omega)\det(\langle\nabla\Phi^i(\omega), \nabla\Phi^j(\omega)\rangle)^{1/2}\,\mathrm{d}\mu_S(\omega)$$

The following co-area formula on the Wiener space

$$\int_X f(\Phi(\omega))F(\omega)(\det\Phi)(\omega)\,\mathrm{d}\mu(\omega) = \int_{\mathbb{R}^d} f(\lambda)\int_{\mathcal{S}_\lambda} F^*(\omega)\,\mathrm{d}\aleph(\omega)\,\mathrm{d}\lambda$$

was proved in Airault and Malliavin (1988).

Calculus of Variations in a Non-Euclidean Setting

Let M be a d-dimensional compact Riemannian manifold with metric $\mathrm{d}s^2 = \sum_{i,j} g_{i,j}\,\mathrm{d}m^i\,\mathrm{d}m^j$. The Laplace–Beltrami operator is expressed in the local chart by

$$\Delta_M = g^{i,j}\frac{\partial^2 f}{\partial m^i\partial m^j} - g^{i,j}\Gamma^k_{i,j}\frac{\partial f}{\partial m^k}$$

where $\Gamma^k_{i,j}$ are the Christoffel symbols associated with the Levi-Civita connection. The corresponding Brownian motion p_w is locally expressed as a solution of the SDE:

$$\mathrm{d}p^i(t) = a^{i,j}(p(t))\,\mathrm{d}W_j(t) - \tfrac{1}{2}g^{j,k}\Gamma^i_{j,k}(p(t))\,\mathrm{d}t$$

with $p(0) = m_0 \in M$ and where $a = \sqrt{g}$. Its law on the space of paths $\mathbb{P}(M) = \{p : [0,1] \to M, p \text{ continuous}, p(0) = m_0\}$ will be denoted by ν.

How can we develop differential calculus and geometry on the space $\mathbb{P}(M)$? An infinite-dimensional local chart approach is delicate, due to the difficulty of finding an atlas in which the changes of charts preserve the measures. A possibility, developed in Cruzeiro and Malliavin (1996), consists in replacing the local chart approach by the Cartan-like methodology of moving frames. The canonical moving

frame in this framework is provided by Itô stochastic parallel transport. Nevertheless, a new difficulty arises: the parallel transport will not be differentiable in the Cameron–Martin sense described before.

Recall that a frame above m is a Euclidean isometry $r: \mathbb{R}^d \to T_m(M)$ onto the tangent space. $O(M)$ denotes the collection of all frames above M and $\pi(r) = m$ the canonical projection. $O(M)$ can be viewed as a parallelized manifold for there exist canonical differential forms (θ, ω) realizing for every r an isomorphism between $T_r(O(M))$ and $\mathbb{R}^d \times \mathrm{so}(d)$.

If $A_\alpha, \alpha = 1, \ldots, d$, denote the horizontal vector fields, which are defined by $<\theta, A_\alpha> = \varepsilon_\alpha$, $<\omega, A_\alpha> = 0$, where ε_α are the vectors of the canonical basis of $\mathbb{R}^d$, then the horizontal Laplacian in $O(M)$ is the operator

$$\Delta_{O(M)} = \sum_{\alpha=1}^{d} A_\alpha^2$$

and we have $\Delta_{O(M)}(f o \pi) = (\Delta_M f) o \pi$. With the Laplacians on M and on $O(M)$ inducing two probability measures, the canonical projection realizes an isomorphism between the corresponding probability spaces.

The Stratonovich SDE

$$\mathrm{d}r_\omega = \sum_\alpha A_\alpha(r_\omega) o\, \mathrm{d}\omega^\alpha, \quad r_\omega(0) = r_0$$

with $\pi(r_0) = m_0$ defines the lifting to $O(M)$ of the Itô parallel transport along the Brownian curve and we write $t^p_{\tau \leftarrow 0} r_0 = r_\omega(\tau)$. Itô map was defined by Malliavin as the map $I: X \to \mathbb{P}(M)$ given by

$$I(\omega)(\tau) = \pi(r_\omega(\tau))$$

This map is a.s. bijective and we have $\nu = \mu \circ I^{-1}$; therefore, it provides an isomorphism of measures from the curved path space to the "flat" Wiener space.

For a cylindrical functional $F = f(p(\tau_1), \ldots, p(\tau_m))$ on $\mathbb{P}(M)$, the derivatives are defined by

$$D_{\tau,\alpha} F(p) = \sum_{k=1}^{m} \mathbf{1}_{\tau < \tau_k} (t^p_{0 \leftarrow \tau_k} (\partial_k F) | \varepsilon_\alpha)$$

The derivative operator is closable in a suitable Sobolev space.

It would be reasonable to think that the differentiable structure considered in the Wiener space would be conserved through the isomorphism I and that the tangent space of $\mathbb{P}(M)$ would consist of transported vectors from the tangent space to X, namely Cameron–Martin vectors. Let us take a map $Z_p(\tau) \in T_{p(\tau)}(M)$ such that $z(\tau) = t^p_{0 \leftarrow \tau} Z_p(\tau)$ belongs to the Cameron–Martin space $\mathcal{H}$.

In order to transfer derivatives to the Wiener space, we need to differentiate the Itô map. We have (Cruzeiro and Malliavin (1996)):

Theorem *The Jacobian matrix of the flow* $r_0 \to r_\omega(\tau)$ *is given by the linear map* $J_{\omega,\tau} = (J^1_{\omega,\tau}, J^2_{\omega,\tau}) \in \mathrm{GL}(\mathbb{R}^d \times \mathrm{so}(d))$ *defined by the system of Stratonovich SDE's*

$$\mathrm{d}_\tau J^1_{\omega,\tau} = \sum_{\alpha=1}^{d} \left(J^1_{\omega,\tau}\right)_\alpha o\, \mathrm{d}\omega_\alpha(\tau)$$

$$\mathrm{d}_\tau J^2_{\omega,\tau} = \sum_{\alpha=1}^{d} \Omega\left(J^1_{\omega,\tau}, \varepsilon_\alpha\right) o\, \mathrm{d}\omega_\alpha(\tau)$$

where Ω denotes the curvature tensor of the underlying manifold read on the frame bundle.

From this result we can deduce the behavior of the derivatives transferred to the Wiener space, a result whose origin is due to B Driver. We have, for a "vector field" $Z_p(\tau)$ on $\mathbb{P}(M)$ as above,

$$(D_Z F) o I = D_\xi(F o I)$$

with ξ solving

$$\mathrm{d}\xi(\tau) = \dot{z}(\tau)\, \mathrm{d}\tau + \rho o\, \mathrm{d}\omega(\tau)$$
$$\mathrm{d}\rho(\tau) = \Omega(o\, \mathrm{d}\omega(\tau), z(\tau))$$

The process ξ is no longer Cameron–Martin space valued. Nevertheless, it satisfies an SDE with an antisymmetric diffusion coefficient (given by the curvature) and therefore, by Levy's theorem, it still corresponds to a transformation of the Wiener space that leaves the measure quasi-invariant. We extend, accordingly, the notion of tangent space in the Wiener space to include processes of the form $\mathrm{d}\xi^\alpha = a^\alpha_\beta \,\mathrm{d}\omega^\beta + c^\alpha \,\mathrm{d}\tau$, with $a^\alpha_\beta + a^\beta_\alpha = 0$. These were called "tangent processes" in Cruzeiro and Malliavin (1996).

Another important consequence of the last theorem is the integration-by-parts formula in the curved setting, initially proved by Bismut (1984):

$$E_\nu(D_Z F) = E_\mu\left((F o I) \int_0^1 [\dot{z} + \tfrac{1}{2}\mathrm{Ricci}(z)]\, \mathrm{d}\omega(\tau)\right)$$

where Ricci is the Ricci tensor of M read on the frame bundle.

Some Applications

We already mentioned that Malliavin calculus has been applied to various domains connected with physics. We shall describe here some of its relations with elementary quantum mechanics.

Feynman gave a path space formulation of quantum theory whose fundamental tool is the concept of transition element of a functional $F(\omega)$ between any two L^2-states ψ_s and ϕ_u, for paths ω defined on a time interval $[s,u]$:

$$<F>_S \equiv <\phi|F|\psi>_S = \int\int\int_\Omega \psi_s(x) \exp\left(\frac{\mathrm{i}}{\hbar} S_L(\omega, u-s)\right) \times F(\omega)\bar{\phi}_u(z)\mathcal{D}\omega \,\mathrm{d}x \,\mathrm{d}z \qquad [6]$$

This is a shorthand for the time discretization version along broken paths ω interpolating linearly between point $x_j = \omega(t_j)$, $t_j = j(u-s)/N$, $j = 0, 1, \ldots, N$. In [6] $\hbar$ is Planck's constant and $S = S_L$ denotes the action functional with Lagrangian L of the underlying classical system. For a particle with mass m in a scalar potential V on the real line,

$$S_L(\omega, u-s) = \int_s^u \left(\frac{m}{2}\dot{\omega}^2(\tau) - V(\omega(\tau))\right) \mathrm{d}\tau \qquad [7]$$

The "$\mathcal{D}\omega$" of [6] is used as a Lebesgue measure, although there is no such thing in infinite dimensions. More generally, the construction of measures or integrals on the various path spaces required for general quantum systems is still nowadays a field of investigation.

When $F = 1$ and $\bar{\phi}_u$ (the complex conjugate of ϕ_u) reduces to a Dirac mass at z, [6] is the path-integral representation of the solution $\psi(x,u)$ of the initial-value problem in L^2:

$$\mathrm{i}\hbar \frac{\partial \psi}{\partial u} = H\psi, \qquad \psi(x,s) = \psi_s(x) \qquad [8]$$

where $H = -(\hbar^2/2)\Delta + V$ and when S_L is as in [7]. Feynman's framework is time symmetric on I: when $\psi_s = \delta_x$ (still for $F = 1$), [6] provides a path-integral representation of the solution of the final-value problem for $\bar{\phi}(z,s)$.

According to Feynman, "it would be possible to use the integration-by-parts formula

$$\left\langle \frac{\delta F}{\delta \omega(s)} \right\rangle = -\frac{\mathrm{i}}{\hbar} \left\langle F \frac{\delta S}{\delta \omega(s)} \right\rangle \qquad [9]$$

as a starting point to define the laws of quantum mechanics" (Feynman and Hibbs 1965, p. 173). The functional derivative corresponds to variations of the underlying paths in directions $\delta\omega$ and

$$\delta F = \int \frac{\delta F}{\delta \omega(s)} \delta\omega(s) \,\mathrm{d}s$$

to an L^2 analog of [4].

Its first consequence, when $F = 1$, is the path space counterpart of Newton's law, in the elementary case [7],

$$<m\ddot{\omega}>_{S_L} = - <\nabla V(\omega)>_{S_L} \qquad [10]$$

where the left-hand side involves a time discretization of the second derivative. When $F(\omega) = \omega(t)$, Feynman obtains the path space version of Heisenberg commutation relation between position and momentum observables:

$$\left\langle \omega(t) \frac{\omega(t) - \omega(t-\epsilon)}{\epsilon} \right\rangle_{S_L} - \left\langle \frac{\omega(t+\epsilon) - \omega(t)}{\epsilon} \omega(t) \right\rangle = \mathrm{i}\frac{\hbar}{m} \qquad [11]$$

and from this the crucial fact that "quantum mechanical paths are very irregular. However, these irregularities average out over a reasonable length of time to produce a reasonable drift or average velocity" (Feynman and Hibbs 1965, p. 177).

A probabilistic interpretation (cf. Cruzeiro and Zambrini (1991)) of Feynman's calculus uses (Bernstein) diffusion processes solving the SDE

$$\mathrm{d}z(t) = \left(\frac{\hbar}{m}\right)^{1/2} \mathrm{d}W(t) + \frac{\hbar}{m} \nabla \log \eta(z(t), t) \,\mathrm{d}t \qquad [12]$$

where the drift stems from a positive solution of the Euclidean version of the above final-value problem for $\bar{\phi}$,

$$\hbar \frac{\partial \eta}{\partial t} = H\eta, \qquad \eta(x,u) = \eta_u(x) \qquad [13]$$

For any regular function f, we can make sense of the "continuous limit"

$$\mathbb{D}f(z(t),t) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} E_t[f(z(t+\epsilon), t+\epsilon) - f(z(t),t))] \qquad [14]$$

where E_t denotes conditional expectation with respect to the past $\mathcal{P}_t$ and check, indeed, that

$$\mathbb{D}z(t) = \frac{\hbar}{m} \nabla \log \eta(z(t), t)$$

is Feynman's "reasonable drift." Using Feynman–Kac formula, one shows that the diffusions [12] have laws which are absolutely continuous with respect to the Wiener measure of parameter $\hbar/m$, with Radon–Nikodym density given by

$$\rho(z) = \frac{\eta(z(u),u)}{\eta(z(s),s)} \exp\left(-\frac{1}{\hbar}\int_0^1 V(z(\tau))\,\mathrm{d}\tau\right)$$

We can, therefore, use Malliavin calculus on the path space of these diffusions and the associated integration-by-parts formula to make sense of [9] and all its consequences.

The probabilistic counterpart of the time symmetry of Feynman's framework is interesting: Heisenberg's original argument to deny the existence of quantum trajectories (1927) was that any position can be associated with two velocities. Feynman's interpretation [11] and the definition [14] suggest that this has to do with a past or future conditioning at time t. Indeed, there is another description of diffusions $z(t)$ with respect to a family of future σ-fields, using the Euclidean version of the initial-value problem for ψ, underlying [6]. Another drift built on the model of the drift in [12] results, and Feynman's commutation relation [11] becomes rigorous (without, of course, the factor i).

We refer to Cruzeiro and Zambrini (1991) for a development of this approach using Malliavin calculus.

See also: Euclidean Field Theory; Functional Integration in Quantum Physics; Measure on Loop Spaces; Stochastic Differential Equations; Stochastic Hydrodynamics.

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Marsden–Weinstein Reduction *see* Cotangent Bundle Reduction; Poisson Reduction; Symmetry and Symplectic Reduction

Maslov Index *see* Optical Caustics; Semiclassical Spectra and Closed Orbits; Stationary Phase Approximation

Mathai–Quillen Formalism

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Introduction

Characteristic classes play an essential role in the study of global properties of vector bundles. Particularly important is the Euler class of real orientable vector bundles. A de Rham representative of the Euler class (for tangent bundles) first appeared in Chern's generalization of the Gauss–Bonnet theorem to higher dimensions. The representative is the Pfaffian of the curvature, whose cohomology class does not depend on the choice of connections. The Euler class of a vector bundle is also the obstruction to the existence of a nowhere-vanishing section. In fact, it is the Poincaré dual of the zero set of any section which intersects the zero section transversely. In the case of tangent bundles, it counts (algebraically) the zeros of a vector field on the manifold. That this is equal to the Euler characteristic number is known as the Hopf theorem. Also significant is the Thom class of a vector bundle: it is the Poincaré dual of the zero section in the total space. It induces, by a cup product, the Thom isomorphism between the cohomology of the base space and that of the total space with compact vertical support. Thom isomorphism also exists and plays an important role in K-theory.

Mathai and Quillen (1986) obtained a representative of the Thom class by a differential form on the total space of a vector bundle. Instead of having a compact support, the form has a nice Gaussian peak near the zero section and exponentially decays along the fiber directions. The pullback of Mathai–Quillen's Thom form by any section is a representative of the Euler class. By scaling the section, one obtains an interpolation between the Pfaffian of the curvature, which distributes smoothly on the manifold, and the Poincaré dual of the zero set, which localizes on the latter. This elegant construction proves to be extremely useful in many situations, from the study of Morse theory, analytic torsion in mathematics to the understanding of topological (cohomological) field theories in physics.

In this article, we begin with the construction of Mathai–Quillen's Thom form. We also consider the case with group actions, with a review of equivariant cohomology and then Mathai–Quillen's construction in this setting. Next, we show that much of the above can be formulated as a "field theory' on a superspace of one fermionic dimension. Finally, we present the interpretation of topological field theories using the Mathai–Quillen formalism.

Mathai–Quillen's Construction

Berezin Integral and Supertrace

Let V be an oriented real vector space of dimension n with a volume element $\nu \in \wedge^n V$ compatible with the orientation. The "Berezin integral" of a form $\omega \in \wedge^* V^*$ on V, denoted by $\int^{\mathrm{B}} \omega$, is the pairing $\langle \nu, \omega \rangle$. Clearly, only the top degree component of ω contributes. For example, if $\sigma \in \wedge^2 V^*$ is a 2-form, then

$$\int^{\mathrm{B}} \mathrm{e}^{\sigma} = \begin{cases} \left\langle \nu, \dfrac{\sigma^{\wedge(n/2)}}{(n/2)!} \right\rangle, & \text{if } n \text{ is even} \\ 0, & \text{if } n \text{ is odd} \end{cases}$$

If V has a Euclidean metric $(\cdot\,,\cdot)$, then ν is chosen to be of unit norm. If $\Sigma \in \mathrm{End}(V)$ is skew-symmetric, then $(1/2)(\cdot\,,\Sigma\,\cdot)$ is a 2-form and, if n is even, the Pfaffian of Σ is

$$\mathrm{Pf}(\Sigma) = \int^{\mathrm{B}} \exp\left(\frac{1}{2}(\cdot\,,\Sigma\,\cdot)\right)$$

The Berezin integral can be defined on elements in a graded tensor product $\wedge^* V^* \hat{\otimes} A$, where A is any $\mathbb{Z}_2$-graded commutative algebra. For example, if we consider the identity operator $\boldsymbol{x} = \mathrm{id}_V$ as a V-valued function on V, then $\mathrm{d}\boldsymbol{x}$ is a 1-form on V valued in V, and $(\mathrm{d}\boldsymbol{x}, \cdot)$ is a 1-form valued in V^*. Let $\{e_1, \ldots, e_n\}$ be an orthonormal basis of V and write $\boldsymbol{x} = x^i e_i$, where x^i are the coordinate functions on V. We let

$$u(\boldsymbol{x}) = \frac{(-1)^{n(n+1)/2}}{(2\pi)^{n/2}} \int^{\mathrm{B}} \exp\left(-\frac{1}{2}(\boldsymbol{x}, \boldsymbol{x}) - (\mathrm{d}\boldsymbol{x}, \cdot)\right)$$

The integrand is in $\Omega^*(V) \hat{\otimes} \wedge^* V^*$. The result is

$$u(\boldsymbol{x}) = \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}, \boldsymbol{x})\right) \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n \quad [1]$$

a Gaussian n-form whose (usual) integration on V is 1.

Let $\mathrm{Cl}(V)$ be the Clifford algebra of V. For any orthonormal basis $\{e_i\}$, let γ^i be the corresponding generators of $\mathrm{Cl}(V)$ and let $\gamma = e_i \otimes \gamma^i \in V \otimes \mathrm{Cl}(V)$. For any $\omega \in \wedge^k V^*$, we have

$$\omega(\gamma, \ldots, \gamma) = \frac{1}{k!} \omega_{i_1 \cdots i_k} \gamma^{i_1} \cdots \gamma^{i_k} \in \mathrm{Cl}(V)$$

If n is even, the Clifford algebra has a unique $\mathbb{Z}_2$-graded irreducible spinor representation $S(V) = S^+(V) \oplus S^-(V)$. For any element $a \in \mathrm{Cl}(V)$, the

supertrace is $\operatorname{str} a = \operatorname{tr}_{S^+(V)} a - \operatorname{tr}_{S^-(V)} a$. If $\Sigma \in \operatorname{End}(V)$ is skew-symmetric, then

$$\operatorname{str}\exp\left(\frac{\sqrt{-1}}{4}(\gamma,\Sigma\gamma)\right) = \hat{A}(\Sigma)^{-1/2}\operatorname{Pf}(\Sigma)$$

where

$$\hat{A}(\Sigma) = \det\left(\frac{\Sigma/2}{\sinh(\Sigma/2)}\right)$$

More generally, supertrace can be defined on $\operatorname{Cl}(V)\hat{\otimes} A$ for any $\mathbb{Z}_2$-graded commutative algebra $A = A^+ \oplus A^-$. If Σ is skew-symmetric and $\alpha \in V^* \otimes A^-$, then

$$\operatorname{str}\exp\left(\frac{\sqrt{-1}}{4}(\gamma,\Sigma\gamma) + \left(\frac{\sqrt{-1}}{2}\right)^{1/2}\alpha(\gamma)\right) = \hat{A}(\Sigma)^{-1/2}\int^{\mathrm{B}}\exp\left(\frac{1}{2}(\cdot,\Sigma\cdot)+\alpha\right) \quad [2]$$

Representatives of the Euler and Thom Classes

Let M be a smooth manifold and let $\pi: E \to M$ be an oriented real vector bundle of rank r. Suppose E has a Euclidean structure $(\cdot,\cdot)$ and ∇ is a compatible connection. The curvature $R \in \Omega^2(M, \operatorname{End}(E))$ is skew-symmetric, and hence $(\cdot, R\,\cdot) \in \Omega^2(M, \wedge^2 E^*)$. A de Rham representative of the Euler class of E is

$$e_\nabla(E) = \frac{1}{(2\pi)^{r/2}}\int^{\mathrm{B}}\exp\left(\frac{1}{2}(\cdot,R\,\cdot)\right) = \operatorname{Pf}\left(\frac{R}{2\pi}\right) \quad [3]$$

Here, the Berezin integration is fiberwise in E: it is the pairing between the integrand and the unit section ν of the trivial line bundle $\wedge^r E$ that is consistent with the orientation of E. The de Rham cohomology class of [3] is independent of the choice of $(\cdot,\cdot)$ or ∇.

Let s be a section of E. Following Berline *et al.* (1992) and Zhang (2001), we consider

$$\mathfrak{s}_{\nabla,s} = \tfrac{1}{2}(s,s) + (\nabla s,\cdot) + \tfrac{1}{2}(\cdot,R\,\cdot) \quad [4]$$

a differential form on M valued in $\wedge^* E^*$. Mathai–Quillen's representative of the Euler class is

$$e_{\nabla,s}(E) = \frac{(-1)^{r(r+1)/2}}{(2\pi)^{r/2}}\int^{\mathrm{B}} \mathrm{e}^{-\mathfrak{s}_{\nabla,s}} \quad [5]$$

One can show that $e_{\nabla,s}(E)$ is closed and that as β varies, the cohomology class of $e_{\nabla,\beta s}(E)$ does not change. By taking $\beta \to 0$, the de Rham class of $e_{\nabla,s}(E)$ is equal to that of $e_\nabla(E)$ when r is even. The form $e_{\nabla,\beta s}(E)$ provides a continuous interpolation between [3] and the limit as $\beta \to \infty$, when the form is concentrated on the zero locus of the section s. In fact, the Euler class is the Poincaré dual to the homology class represented by $s^{-1}(0)$. Hence, if $n \geq m$ and if $\omega \in \Omega^{n-m}(M)$ is closed, we have

$$\int_M \omega \wedge e_{\nabla,s}(E) = \int_{s^{-1}(0)} \omega \quad [6]$$

when s intersects the zero section transversely.

To obtain Mathai–Quillen's representative of the Thom class, we consider the pullback of E to E itself. The bundle $\pi^*E \to E$ has a tautological section $\boldsymbol{x}$. Applying [5] to this setting, we get

$$\tau_\nabla(E) = \frac{(-1)^{r(r+1)/2}}{(2\pi)^{r/2}}\int^{\mathrm{B}}\exp\left(-\frac{1}{2}(\boldsymbol{x},\boldsymbol{x}) - (\nabla\boldsymbol{x},\cdot) - \frac{1}{2}(\cdot,R\,\cdot)\right) \quad [7]$$

where $(\cdot,\cdot)$, ∇, and R are understood to be the pullbacks to π^*E. This is a closed form on the total space of E. Moreover, its restriction to each fiber is the Gaussian form [1]. The cohomology groups of differential forms with exponential decay along the fibers are isomorphic to those with compact vertical support or the relative cohomology groups $H^*(E, E\setminus M)$. Here M is identified with its image under the inclusion $i: M \to E$ by the zero section. Under the above isomorphism, the cohomology class represented by $\tau_\nabla(E)$ coincides with the Thom class $\tau(E) = i_*1 \in H^r(E, E\setminus M)$ defined topologically. For any section $s \in \Gamma(E)$, we have $e_{\nabla,s}(E) = s^*\tau_\nabla(E)$.

Character Form of the Thom Class in *K*-Theory

Let $E = E^+ \oplus E^-$ be a $\mathbb{Z}_2$-graded vector bundle over M. The spaces $\Omega^*(M,E)$, $\Gamma(\operatorname{End}(E))$ and $\Omega^*(M)\hat{\otimes}\Gamma(\operatorname{End}(E))$ are also $\mathbb{Z}_2$-graded. The action of $\alpha\hat{\otimes} T \in \Omega^*(M)\hat{\otimes}\Gamma(\operatorname{End}(E))$ on $\beta\otimes s \in \Omega^*(M,E)$ is

$$\alpha\hat{\otimes}T : \beta\otimes s \mapsto (-1)^{|T||\beta|}(\alpha\wedge\beta)\otimes(Ts)$$

The supertrace of $A \in \Gamma(\operatorname{End}(E))$ is $\operatorname{str} A = \operatorname{tr}_{E^+} A - \operatorname{tr}_{E^-} A$; it extends $\Omega^*(M)$-linearly to $\operatorname{str}: \Omega^*(M)\hat{\otimes}\Gamma(\operatorname{End}(E)) \to \Omega^*(M)$. Let ∇ be a connection on E preserving the grading. ∇ is an odd operator on $\Omega^*(M,E)$. If $L \in \Gamma(\operatorname{End}(E)^-)$ is odd, then $D = \nabla + L$ is called a "superconnection" on E; the "curvature" $D^2 = R + \nabla L + L^2 \in (\Omega^*(M)\otimes\Gamma(\operatorname{End}(E)))^+$ is even. With the superconnection, the Chern character of the virtual vector bundle $E^+ \ominus E^-$ can be represented by

$$\operatorname{ch}_{\nabla,L}(E^+, E^-) = \operatorname{str}\exp\left(\frac{\sqrt{-1}}{2\pi}D^2\right) \quad [8]$$

It is a closed form on M and its de Rham cohomology class is independent of the choice of ∇ or L. If L is invertible everywhere on M and the eigenvalues of $\sqrt{-1}L^2$ are negative, then [8] is exact:

$$\mathrm{ch}_{\nabla,L}(E^+,E^-) = -\frac{\sqrt{-1}}{2\pi}\,\mathrm{d}\int_1^\infty \mathrm{str}\left(\exp\left(\frac{\sqrt{-1}}{2\pi}(\nabla+\beta L)^2\right)L\right)\mathrm{d}\beta$$

Now let E be an oriented real vector bundle of rank $r=2m$ over M with a Euclidean structure $(\cdot,\cdot)$. Suppose further that E has a spin structure. The associated spinor bundle $S(E)=S^+(E)\oplus S^-(E)$ is a graded complex vector bundle over M. For any section $s\in\Gamma(E)$, let $c(s)\in\Gamma(\mathrm{End}(E)^-)$ be the Clifford multiplication on E. Then for any $s,s'\in\Gamma(E)$, we have $\{c(s),c(s')\}=-2(s,s')$. Given a connection ∇ on E preserving $(\cdot,\cdot)$, the induced spinor connection ∇^S on $S(E)$ preserves the grading. If R is the curvature of ∇, that of ∇^S is $R^S=-(1/4)\,(\gamma,R\gamma)$, where γ is now a section of $E\otimes\mathrm{Cl}(E)$. For any $s\in\Gamma(E)$, consider the superconnection

$$D_s=\nabla^S+\left(\frac{\pi}{\sqrt{-1}}\right)^{1/2}c(s)$$

The Chern character form [8] of $S^+(E)\ominus S^-(E)$ is, using [2],

$$\mathrm{ch}_{\nabla,s}(S^+(E),S^-(E))=(-1)^m\hat{A}\left(\frac{R}{2\pi}\right)^{-1/2}e_{\nabla,s}(E)\qquad[9]$$

where $e_{\nabla,s}(E)$ is given by [5]. In cohomology groups, [9] reduces to

$$\mathrm{ch}(S^+(E))-\mathrm{ch}(S^-(E))=(-1)^m\hat{A}(E)^{-1/2}e(E)$$

If M is noncompact and the norm of s increases rapidly away from $s^{-1}(0)$, then both sides of [9] are differential forms that decay rapidly away from $s^{-1}(0)$ and can represent cohomology classes of such. As before, we take the pullback π^*E with the tautological section $\boldsymbol{x}$. Then [9] becomes

$$\mathrm{ch}_\nabla(\pi^*S^+(E),\pi^*S^-(E)) = (-1)^m\pi^*\hat{A}\left(\frac{R}{2\pi}\right)^{-1/2}\tau_\nabla(E)\qquad[10]$$

where $\tau_\nabla(E)$ is given by [7]. Both sides of [10] are forms on E that decays exponentially in the fiber directions; hence, it descends to an equality in $H^*(E,E\backslash M)$. In the relative K-group $K(E,E\backslash M)$, the pair $\pi^*S^\pm(E)$ with the isomorphism $c(\boldsymbol{x})$ away form the zero section is, up to a factor of $(-1)^m$, the K-theoretic Thom class $i_!1\in K(E,E\backslash M)$. Therefore, [10] reduces to the well-known formula

$$\mathrm{ch}(i_!1)=\pi^*\hat{A}(E)^{-1/2}i_*1$$

in cohomology groups $H^*(E,E\backslash M)$. The refinement [10] as an equality of differential forms is due to Mathai and Quillen (1986). In fact, this is how [7] was derived originally.

Equivariant Cohomology and Equivariant Vector Bundles

Equivariant Cohomology

Let G be a compact Lie group with Lie algebra $\mathfrak{g}$. Fixing a basis $\{e_a\}$ of $\mathfrak{g}$, the structure constants are given by $[e_a,e_b]=t^c_{ab}e_c$. Let $\{\vartheta^a\}$ and $\{\varphi^a\}$ be the dual bases of $\mathfrak{g}^*$ generating the exterior algebra $\wedge(\mathfrak{g}^*)$ and the symmetric algebra $S(\mathfrak{g}^*)$, respectively. The Weil algebra is $W(\mathfrak{g})=\wedge(\mathfrak{g}^*)\hat{\otimes}S(\mathfrak{g}^*)$. We define a grading on $W(\mathfrak{g})$ by specifying $\deg\vartheta^a=1,\deg\varphi^a=2$. The contraction ι_a and the exterior derivative d are two odd derivations on $W(\mathfrak{g})$ defined by

$$\begin{aligned}\iota_a\vartheta^b&=\delta^b_a, & \iota_a\varphi^b&=0\\ \mathrm{d}\vartheta^a&=-\tfrac{1}{2}t^a_{bc}\vartheta^b\vartheta^c+\varphi^a, & \mathrm{d}\varphi^a&=-t^a_{bc}\vartheta^b\varphi^c\end{aligned}\qquad[11]$$

The Lie derivative is $L_a=\{\iota_a,d\}$. These operators satisfy the usual (anti-)commutation relations

$$d^2=0,\qquad L_a=\{\iota_a,d\},\qquad [L_a,d]=0\qquad[12]$$

$$\begin{aligned}\{\iota_a,\iota_b\}=0,\qquad [L_a,\iota_b]=t^c_{ab}\iota_c,\\ [L_a,L_b]=t^c_{ab}L_c\end{aligned}\qquad[13]$$

The cohomology of $(W(\mathfrak{g}),d)$ is trivial.

If G acts smoothly on a manifold M on the left, let V_a be the vector field generated by the Lie algebra element $-e_a\in\mathfrak{g}$. Then, $[V_a,V_b]=t^c_{ab}V_c$. Denote $\iota_a=\iota_{V_a}$ and $L_a=L_{V_a}$, acting on $\Omega^*(M)$. In the Weil model of equivariant cohomology, one considers the graded tensor product $W(\mathfrak{g})\hat{\otimes}\Omega^*(M)$, on which the operators

$$\begin{aligned}\tilde{\iota}_a&=\iota_a\hat{\otimes}1+1\hat{\otimes}\iota_a\\ \tilde{d}&=d\hat{\otimes}1+1\hat{\otimes}d\\ \tilde{L}_a&=L_a\hat{\otimes}1+1\hat{\otimes}L_a\end{aligned}$$

act and satisfy the same relations [12] and [13]. An element $\omega\in W(\mathfrak{g})\hat{\otimes}\Omega^*(M)$ is "basic" if it satisfies $\iota_a\omega=0,L_a\omega=0$ for all indices a. Let $\Omega^*_G(M)=(W(\mathfrak{g})\hat{\otimes}\Omega^*(M))_{\mathrm{bas}}$ be the set of such. Elements of $\Omega^*_G(M)$ are equivariant differential forms on M. The operator $\tilde{d}$ preserves $\Omega^*_G(M)$ and its cohomology groups $H^*_G(M)$ are the equivariant cohomology groups of M. They are

isomorphic to the singular cohomology groups of $EG \times_G M$ with real coefficients.

The BRST model of Kalkman (1993) is obtained by applying an isomorphism $\sigma = e^{\vartheta^a \otimes \iota_a}$ of $W(\mathfrak{g}) \hat{\otimes} \Omega^*(M)$. The operators become

$$\sigma \circ \tilde{\iota}_a \circ \sigma^{-1} = \iota_a \hat{\otimes} 1$$
$$\sigma \circ \tilde{d} \circ \sigma^{-1} = \tilde{d} - \varphi^a \hat{\otimes} \iota_a + \vartheta^a \hat{\otimes} L_a$$
$$\sigma \circ \tilde{L}_a \circ \sigma^{-1} = \tilde{L}_a$$

The subspace of basic forms in the Weil model becomes

$$\sigma(\Omega^*_G(M)) = (S(\mathfrak{g}^*) \otimes \Omega^*(M))^G$$

This is precisely the Cartan model of equivariant cohomology, in which the exterior differential is

$$\tilde{d}' = 1 \otimes d - \varphi^a \otimes \iota_a$$

If P is a principal G-bundle over a base space B, we can form an associated bundle $P \times_G M \to B$. Choose a connection on P and let $\Theta = \Theta^a e_a \in \Omega^1(P) \otimes \mathfrak{g}, \Phi = \Phi^a e_a \in \Omega^2(P) \otimes \mathfrak{g}$ be the connection and curvature forms, respectively. The components Θ^a, Φ^a satisfy the same relations [11]. Replacing ϑ^a, φ^a by Θ^a, Φ^a, we have a homomorphism that maps $\omega \in W(\mathfrak{g}) \otimes \Omega^*(M)$ to $\hat{\omega} \in \Omega^*(P \times M)$. If ω is basic, then so is $\hat{\omega}$, and the latter descends to a form $\bar{\omega}$ on $P \times_G M$. Furthermore, the operator $\tilde{d}$ on $\Omega^*_G(M)$ descends to d on $\Omega^*(P \times_G M)$. Thus, we get the Chern–Weil homomorphisms $\Omega^*_G(M) \to \Omega^*(P \times_G M)$ and $H^*_G(M) \to H^*(P \times_G M)$. For example, the vector space $\mathbb{R}^r$ has an obvious SO(r) action. The Gaussian r-form [1] is invariant under SO(r) and can be extended to an SO(r)-equivariant closed r-form, called the "universal Thom form." Let E be an orientable real vector bundle E of rank r with a Euclidean structure. E determines a principal SO(r)-bundle P; the associated bundle $P \times_{SO(r)} \mathbb{R}^r$ is E itself. By applying the Chern–Weil homomorphism to this setting, we get a closed r-form on E. This is another construction of the Thom form [7] by Mathai and Quillen (1986). Further information of equivariant cohomology can be found there, and in Berline *et al.* (1992) and Guillemin and Sternberg (1999).

Equivariant Vector Bundles

Recall that a connection on a vector bundle $E \to M$ determines, for any $k \geq 0$, a differential operator

$$\nabla : \Omega^k(M, E) \to \Omega^{k+1}(M, E)$$

The curvature $R = \nabla^2 \in \Omega^2(M, \mathrm{End}(E))$ satisfies the Bianchi identity $\nabla R = 0$. If the connection preserves a Euclidean structure on E, then R is skew-symmetric.

If a Lie group G acts on M and the action can be lifted to E, then G also acts on the spaces $\Gamma(E)$ and $\Omega^*(M, E)$. As before, the Lie derivatives L_a on these spaces are the infinitesimal actions of $-e_a \in \mathfrak{g}$. We choose a G-invariant connection on E. The "moment" of the connection ∇ under the G-action is $\mu_a = L_a - \nabla_{V_a}$ acting on $\Gamma(E)$. In fact, μ_a is a section of End(E), or $\mu \in \Gamma(\mathrm{End}(E)) \otimes \mathfrak{g}^*$. If a Euclidean structure on E is preserved by both the connection and the G-action, then μ_a is skew-symmetric. On $\Omega^*(M, E)$, we have

$$L_a = \{\iota_a, \nabla\} + \mu_a$$
$$\iota_a R = \nabla \mu_a, \qquad L_a \mu_b = t^c_{ab} \mu_c$$
$$[\mu_a, \mu_b] = t^c_{ab} \mu_c + R_{ab}$$

where $R_{ab} = R(V_a, V_b) \in \Gamma(\mathrm{End}(E))$.

On the graded tensor product $W(\mathfrak{g}) \hat{\otimes} \Omega^*(M, E)$, the contraction $\tilde{\iota}_a$ and the Lie derivative $\tilde{L}_a$ act and satisfy [13]. In the Weil model, equivariant differential forms on M with values in E are the basic elements in $W(\mathfrak{g}) \hat{\otimes} \Omega^*(M, E)$, which form a subspace $\Omega^*_G(M, E) = (W(\mathfrak{g}) \hat{\otimes} \Omega^*(M, E))_{\mathrm{bas}}$. The "equivariant covariant derivative" is

$$\tilde{\nabla} = d \hat{\otimes} 1 + 1 \hat{\otimes} \nabla + \vartheta^a \hat{\otimes} \mu_a \qquad [14]$$

One checks that $\{\iota_a, \tilde{\nabla}\} = \tilde{L}_a$ and hence $\tilde{\nabla}$ preserves the basic subspace $\Omega^*_G(M, E)$. The equivariant curvature $\tilde{R} = \tilde{\nabla}^2$ is

$$\tilde{R} = R - \vartheta^a \nabla \mu_a + \varphi^a \mu_a + \tfrac{1}{2} \vartheta^a \vartheta^b R_{ab} \qquad [15]$$

It satisfies the equivariant Bianchi identity $\tilde{\nabla}\tilde{R} = 0$. Equivariant characteristic forms are invariant polynomials of $\tilde{R}$. They are equivariantly closed and their equivariant cohomology classes do not depend on the choice of the G-invariant connection. Hence, they represent the equivariant characteristic classes of E in $H^*_G(M)$.

For the BRST model, we use a similar isomorphism $\sigma = e^{\vartheta^a \otimes \iota_a}$ on $W(\mathfrak{g}) \hat{\otimes} \Omega^*(M, E)$. The operators become

$$\sigma \circ \tilde{\iota}_a \circ \sigma^{-1} = \iota_a \hat{\otimes} 1$$
$$\sigma \circ \tilde{\nabla} \circ \sigma^{-1} = \tilde{\nabla} - \varphi^a \hat{\otimes} \iota_a + \vartheta^a \hat{\otimes} L_a$$
$$\sigma \circ \tilde{L}_a \circ \sigma^{-1} = \tilde{L}_a$$

and the basic subspace turns into

$$\sigma(\Omega^*_G(M, E)) = (S(\mathfrak{g}^*) \otimes \Omega^*(M, E))^G$$

This is the Cartan model, which can be found in Berline *et al.* (1992). The equivariant covariant derivative is

$$\tilde{\nabla}' = 1 \otimes \nabla - \varphi^a \otimes \iota_a$$

The equivariant curvature is $\tilde{R}' = (\tilde{\nabla}')^2 = R + \varphi^a \mu_a$ and the characteristic forms are defined similarly.

Let $P \to B$ be a principal G-bundle with a connection Θ. Following [14], the bundle $P \times E \to P \times M$ has a connection

$$\hat{\nabla} = d \otimes 1 + 1 \otimes \nabla + \Theta^a \otimes \mu_a$$

It descends to a connection $\bar{\nabla}$ on the vector bundle $P \times_G E \to P \times_G M$. The map $\tilde{\nabla} \mapsto \bar{\nabla}$ can be considered as the analog of the Chern–Weil homomorphism for connections. There is also a homomorphism $\Omega^*_G(M, E) \to \Omega^*(P \times_G M, P \times_G E)$, which commutes with the covariant derivatives $\tilde{\nabla}, \bar{\nabla}$. The curvature $\bar{R} = \bar{\nabla}^2$ is the image of the equivariant curvature $\tilde{R}$. Consequently, the equivariant characteristic forms descend to those of $P \times_G E \to P \times_G M$ by the usual Chern–Weil homomorphism.

Now let $E = E^+ \oplus E^-$ be a graded vector bundle over M with a G-action preserving all the structures. We have the $\Omega^*_G(M)$-linear supertrace map str: $\Omega^*_G(M) \hat{\otimes} \Gamma(\mathrm{End}(E)) \to \Omega^*_G(M)$. If ∇ is a G-invariant connection on E preserving the grading and if $L \in \Gamma(\mathrm{End}(E)^-)^G$ is odd and G-invariant, then $\tilde{D} = \tilde{\nabla} + L$ is an "equivariant superconnection." The equivariant counterpart of [8] is

$$\mathrm{ch}_{\tilde{\nabla}, L}(E^+, E^-) = \mathrm{str} \exp\left(\frac{\sqrt{-1}}{2\pi} \tilde{D}^2\right) \in \Omega^*_G(M)$$

representing the equivariant Chern character of $E^+ \ominus E^-$ in $H^*_G(M)$.

Representatives of the Equivariant Euler and Thom Classes

Consider an oriented real vector bundle $E \to M$ of rank r with a Euclidean structure $(\cdot, \cdot)$. Choose a connection ∇ on E preserving $(\cdot, \cdot)$. We assume that a Lie group G acts on M and that the action can be lifted to E preserving all the structures on E. We use the Weil model; the constructions in the Cartan model are similar. For any $\alpha \in \Omega^k_G(M, E)$ and $\beta \in \Omega^l_G(M, E)$, we obtain $(\alpha, \wedge \beta) \in \Omega^{k+l}_G(M)$ by taking the wedge product of forms as well as the pairing in E. The Berezin integral of $\omega \in \Omega^*_G(M, \wedge^* E^*)$ along the fibers of E is $\int^B \omega = \langle \nu, \omega \rangle \in \Omega^*_G(M)$. Here, ν is the unit section of the canonically trivial determinant line bundle $\wedge^r E$, compatible with the orientation of E. The equivariant Euler form

$$e_{\tilde{\nabla}}(E) = \frac{1}{(2\pi)^{r/2}} \int^B \exp\left(\frac{1}{2}(\cdot, \tilde{R} \cdot)\right) = \mathrm{Pf}\left(\frac{\tilde{R}}{2\pi}\right) \quad [16]$$

is equivariantly closed. It represents the equivariant Euler class $e_G(E) \in H^*_G(M)$.

Given a G-invariant section $s \in \Gamma(E)^G$, the equivariant counterpart of [4] is

$$\mathcal{S}_{\tilde{\nabla}, s} = \tfrac{1}{2}(s, s) + (\tilde{\nabla} s, \cdot) + \tfrac{1}{2}(\cdot, \tilde{R} \cdot) \quad [17]$$

and that of Mathai–Quillen's Euler form [5] is

$$e_{\tilde{\nabla}, s}(E) = \frac{(-1)^{r(r+1)/2}}{(2\pi)^{r/2}} \int^B \mathrm{e}^{-\mathcal{S}_{\tilde{\nabla}, s}} \quad [18]$$

It is also equivariantly closed, and its equivariant cohomology class is $e_G(E)$. The equivariant extension of Mathai–Quillen's Thom form [7] is

$$\tau_{\tilde{\nabla}}(E) = \frac{(-1)^{r(r+1)/2}}{(2\pi)^{r/2}} \int^B \exp\left(-\frac{1}{2}(\boldsymbol{x}, \boldsymbol{x}) - (\tilde{\nabla} \boldsymbol{x}, \cdot) - \frac{1}{2}(\cdot, \tilde{R} \cdot)\right) \quad [19]$$

where $\boldsymbol{x}$ is the (G-invariant) tautological section of $\pi^* E \to E$.

Finally, G acts on the (graded) spinor bundle $S(E)$. Using the equivariant superconnection

$$\tilde{D}_s = \tilde{\nabla}^S + \left(\frac{\pi}{\sqrt{-1}}\right)^{1/2} c(s)$$

[9] generalizes to

$$\mathrm{ch}_{\tilde{\nabla}, s}(S^+(E), S^-(E)) = (-1)^m \hat{A}\left(\frac{\tilde{R}}{2\pi}\right)^{-1/2} e_{\tilde{\nabla}, s}(E)$$

Now apply the construction to the bundle $\pi^* E \to E$ and its tautological section $\boldsymbol{x}$. The pair $\pi^* S^{\pm}(E)$ with an odd bundle map $c(\boldsymbol{x})$ determines, up to a factor of $(-1)^m$, the Thom class $i_! 1_G$ in the equivariant K-group $K_G(E, E \backslash M)$. The equivariant analog of [10] descends to

$$\mathrm{ch}_G(i_! 1_G) = \pi^* \hat{A}_G(E)^{-1/2} i_* 1_G$$

in equivariant cohomology.

Superspace Formulation

Mathai–Quillen Formalism and the Superspace $\mathbb{R}^{0|1}$

Let $\mathbb{R}^{0|1}$ be the superspace with one fermionic coordinate θ but no bosonic coordinates. The translation on $\mathbb{R}^{0|1}$ is generated by $D = \partial/\partial\theta$, which satisfies $\{D, D\} = 0$. We consider a sigma model on $\mathbb{R}^{0|1}$ whose target space is an (ordinary) smooth manifold M of dimension n. A map $X: \mathbb{R}^{0|1} \to M$ can be written as $X(\theta) = x + \sqrt{-1}\theta\psi$. Here, $x = X|_{\theta=0} \in M$ and $\psi = -\sqrt{-1} DX|_{\theta=0} \in T_x M$; the latter is fermionic. Under the translation

$\theta \mapsto \theta + \epsilon$, x and ψ vary according to the supersymmetry transformations

$$\begin{aligned} \delta x &= \epsilon DX|_{\theta=0} = \sqrt{-1}\epsilon\psi \\ \delta\psi &= \epsilon D(DX)|_{\theta=0} = 0 \end{aligned} \qquad [20]$$

Clearly, $\delta^2 = 0$, which is also a consequence of $D^2 = 0$.

For any p-form $\omega \in \Omega^p(M)$, we have an observable

$$\mathcal{O}_\omega(X) = \frac{1}{p!} X^*\omega(D, \ldots, D)|_{\theta=0}$$

In local coordinates,

$$\omega = \frac{1}{p!}\omega_{i_1\cdots i_p}(x)\,\mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_p}$$

and

$$\mathcal{O}_\omega(x, \psi) = \frac{\sqrt{-1}^p}{p!}\omega_{i_1\cdots i_p}(x)\psi^{i_1}\cdots\psi^{i_p}$$

Using $C(\,\cdot\,)$ to denote the set of function(al)s on a space, we can identify $C(\mathrm{Map}(\mathbb{R}^{0|1}, M))$ with $\Omega^*(M)$. Under [20], $\delta\mathcal{O}_\omega(X) = \epsilon\mathcal{O}_{d\omega}(X)$. So, $\mathcal{O}_\omega(X)$ is invariant under supersymmetry if and only if ω is closed. The cohomology of δ is the de Rham cohomology of M. Consider the measure $[\mathrm{d}X] = [\mathrm{d}x][\mathrm{d}\psi]$. In local coordinates, $[\mathrm{d}x] = \mathrm{d}x^1 \cdots \mathrm{d}x^n$ is the standard (bosonic) measure and $[\mathrm{d}\psi] = \mathrm{d}\psi^1 \cdots \mathrm{d}\psi^n$ is a fermionic measure such that

$$\int [\mathrm{d}\psi](-1)^{n(n-1)/2}\psi^1\cdots\psi^n = 1$$

For any $\omega \in \Omega^n(M)$, the superfield integral $\int [\mathrm{d}X]\mathcal{O}_\omega(X)$ is equal to the usual integral $\int_M \omega$ if the latter exists.

Let $E \to M$ be a real vector bundle of rank r with an inner product $(\cdot\,,\cdot)$, and let ∇ be a compatible connection whose curvature is R. Consider a theory whose fields are $X \in \mathrm{Map}(\mathbb{R}^{0|1}, M)$ and a fermionic section $\Xi \in \Gamma(X^*E)$. Let $\mathcal{D} = (X^*\nabla)_D$ be the covariant derivative along D in the pullback bundle $X^*E \to \mathbb{R}^{0|1}$. Then, $\chi = \Xi|_{\theta=0} \in E_x$ is fermionic and $f = \mathcal{D}\Xi|_{\theta=0} \in E_x$ is bosonic.

Given a fixed section $s \in \Gamma(E)$, we write a superspace action

$$\begin{aligned} S_{\mathrm{MQ}}[X, \Xi] &= \int_{\mathbb{R}^{0|1}} \mathrm{d}\theta(\Xi, \tfrac{1}{2}\mathcal{D}\Xi + \sqrt{-1}s \circ X) \\ &= \tfrac{1}{2}(f, f) + \sqrt{-1}(f, s) - (\nabla_\psi s, \chi) \\ &\quad + \tfrac{1}{4}(\chi, R(\psi, \psi)\chi) \end{aligned} \qquad [21]$$

It is automatically supersymmetric. Performing the Gaussian integral over f and replacing χ by $-\sqrt{-1}\chi$, we get

$$\int [\mathrm{d}\Xi]\mathrm{e}^{-S_{\mathrm{MQ}}[X,\Xi]} = \frac{\sqrt{-1}^r}{(2\pi)^{r/2}}\int [\mathrm{d}\chi]\,\mathrm{e}^{-S_{\mathrm{MQ}}[x,\psi,\chi]} \qquad [22]$$

where

$$\begin{aligned} &S_{\mathrm{MQ}}[x, \psi, \chi] \\ &= \tfrac{1}{2}(s, s) - \sqrt{-1}(\chi, \nabla_\psi s) - \tfrac{1}{4}(\chi, R(\psi, \psi)\chi) \end{aligned} \qquad [23]$$

When r is even, [22] is equal to $\mathcal{O}_{e(\nabla,s)(E)}(X)$, where $e(\nabla, s)(E)$ is given by [5]. Furthermore, for any closed form ω on M, the expectation value

$$\langle\mathcal{O}_\omega(X)\rangle = \int [\mathrm{d}X][\mathrm{d}\Xi]\mathcal{O}_\omega(X)\,\mathrm{e}^{-S_{\mathrm{MQ}}[X,\Xi]} \qquad [24]$$

is equal to [6].

Equivariant Cohomology and Gauged Sigma Model on $\mathbb{R}^{0|1}$

Suppose G is a Lie group and P is a principal G-bundle over $\mathbb{R}^{0|1}$. Since θ is nilpotent, we can choose a "trivialization" of P such that the connection and curvature are $A \in \Omega^1(\mathbb{R}^{0|1}) \otimes \mathfrak{g}$ and $F \in \Omega^2(\mathbb{R}^{0|1}) \otimes \mathfrak{g}$, respectively. ($\mathfrak{g}$ is the Lie algebra of G.) In components, $c = \sqrt{-1}\iota_D A \in \mathfrak{g}$ is fermionic and $\phi = -(\sqrt{-1}/2)\iota_D^2 F \in \mathfrak{g}$ is bosonic. The space of connections $\mathcal{A}$ is the set of pairs (c, ϕ). Under $\theta \mapsto \theta + \epsilon$,

$$\begin{aligned} \delta c &= \epsilon\left(\phi + \frac{\sqrt{-1}}{2}[c, c]\right) \\ \delta\phi &= \sqrt{-1}\epsilon[c, \phi] \end{aligned} \qquad [25]$$

Thus, the algebra $C(\mathcal{A})$ is isomorphic to the Weil algebra $W(\mathfrak{g})$ and δ corresponds to the differential d in [11]. This relation between gauge theory on a fermionic space and the Weil algebra can be found in Blau and Thompson (1997).

With a trivialization of P, the group of gauge transformation $\mathcal{G}$ can be identified with $\mathrm{Map}(\mathbb{R}^{0|1}, G)$. Any group element is of the form $\hat{g} = g\mathrm{e}^{\sqrt{-1}\xi\theta}$, with $g = \hat{g}|_{\theta=0} \in G$ and $\xi = \sqrt{-1}\iota_D\hat{g}^*\varpi \in \mathfrak{g}$ (fermionic), where ϖ is the Maurer–Cartan form on G. The action of $\hat{g}$ is $A \mapsto A' = \mathrm{Ad}_{\hat{g}}(A - \hat{g}^*\varpi)$, or $c \mapsto c' = \mathrm{Ad}_g(c - \xi)$ and $\phi \mapsto \phi' = \mathrm{Ad}_g\phi$. By choosing $\xi = c$, we obtained a new trivialization, called the "Wess–Zumino gauge," in which $c' = 0$. The residual gauge redundancy is G, and $\mathcal{A}/\mathcal{G} = \mathfrak{g}/\mathrm{Ad}_G$. The Wess–Zumino gauge is not preserved by the translation on $\mathbb{R}^{0|1}$ unless we define δ' by composing δ with a suitable (infinitesimal) gauge transformation. If so, then $\delta'\phi = 0$.

Suppose M is a manifold with a left G-action. As before, let $\{e_a\}$ be a basis of $\mathfrak{g}$ and let the vector field V_a be the infinitesimal action of $-e_a$. In the gauged sigma model, we include another field $X \in \Gamma(P \times_G M)$. With a trivialization of P, we can identify X with a map

$X:\mathbb{R}^{0|1}\to M$. The covariant derivative is given by $\nabla X = \mathrm{d}X - A^a V_a, \mathcal{D}X = \nabla_D X$. Let $x = X|_{\theta=0}\in M$ and $\psi = -\sqrt{-1}\mathcal{D}X|_{\theta=0}\in T_xM$. Then the supersymmetric transformations are

$$\begin{aligned}\delta x^i &= \sqrt{-1}\epsilon\left(\psi^i - c^a V_a^i\right)\\ \delta\psi^i &= -\epsilon\left(\phi^a V_a^i + \sqrt{-1}c^j V_{a,j}^i\right)\end{aligned} \qquad [26]$$

In the Wess–Zumino gauge, the transformations simplify to $\delta' x = \sqrt{-1}\epsilon\psi, \delta'\psi = -\epsilon\phi^a V_a$.

The observables form the $\mathcal{G}$-invariant part of the space $C(\mathcal{A}\times \mathrm{Map}(\mathbb{R}^{0|1}, M))$. For any $\omega\in\Omega^p(M)$, we have

$$\begin{aligned}\mathcal{O}_\omega(X,A) &= \frac{1}{p!}\omega(\mathcal{D}X,\ldots,\mathcal{D}X)|_{\theta=0}\\ &= \frac{\sqrt{-1}^p}{p!}\omega_{i_1\cdots i_p}(x)\psi^{i_1}\cdots\psi^{i_p}\end{aligned} \qquad [27]$$

$\mathcal{O}_\omega(X,A)$ is gauge covariant: $\mathcal{O}_\omega(X,A)\mapsto \mathcal{O}_{g^*\omega}(X,A)$, and the set of gauge-invariant observables is thus identified with $(S(\mathfrak{g}^*)\times\Omega^*(M))^G$. Moreover, since

$$\begin{aligned}\delta\mathcal{O}_\omega(X,A) = \epsilon(&\mathcal{O}_{\mathrm{d}\omega}(X,A) - \sqrt{-1}c^a\mathcal{O}_{L_a\omega}(X,A)\\ &-\sqrt{-1}\phi^a\mathcal{O}_{\iota_a\omega}(X,A))\end{aligned}$$

δ corresponds to the differential $\tilde{d}'$ in BRST model.

Let $E\to M$ be an equivariant vector bundle and let ∇ be a G-invariant connection with curvature R and moment μ. Any $s\in\Gamma(E)^G$ defines a section of $P\times_G E\to P\times_G M$, still denoted by s. Consider a theory with superfields $X\in\Gamma(P\times_G M)$ and $\Xi\in\Gamma(X^*(P\times_G E))$ (fermionic). Let $\mathcal{D}$ be the covariant derivative of the pullback connection. With a trivialization of P, we put $\chi = \Xi|_{\theta=0}\in E_x$ (fermionic) and $f = \mathcal{D}\Xi|_{\theta=0}\in E_x$ (bosonic). The equivariant extension of [21] is

$$S_{\mathrm{MQ}}[X,\Xi,A] = \int_{\mathbb{R}^{0|1}} \mathrm{d}\theta(\Xi, \tfrac{1}{2}\mathcal{D}\Xi + \sqrt{-1}s\circ X)$$

Similar to [22], we get, in the Wess–Zumino gauge,

$$\int[\mathrm{d}\Xi]\mathrm{e}^{-S_{\mathrm{MQ}}[X,\Xi,A]} = \frac{\sqrt{-1}^r}{(2\pi)^{r/2}}\int[\mathrm{d}\chi]\mathrm{e}^{-S_{\mathrm{MQ}}[x,\psi,\phi,\chi]} \qquad [28]$$

where

$$\begin{aligned}&S_{\mathrm{MQ}}[x,\psi,\phi,\chi]\\ &\quad= \frac{1}{2}(s,s) - \sqrt{-1}(\chi,\nabla_\psi s)\\ &\quad\quad -\frac{1}{4}(\chi, R(\psi,\psi)\chi) - \frac{\sqrt{-1}}{2}(\chi,\phi^a\mu_a\chi)\end{aligned} \qquad [29]$$

When r is even, [28] is equal to $\mathcal{O}_{\tilde{e}(\nabla,s)}(X,A)$, where $\tilde{e}(\nabla,s)$ is given by [18].

The Atiyah–Jeffrey Formula

Given the G-action on M, for any $x\in M$, there is a linear map $C_x:\mathfrak{g}\to T_xM$ defined by $C_x(e_a) = V_a(x)$. With an invariant inner product $(\cdot,\cdot)$ on $\mathfrak{g}$ and an invariant Riemannian metric on M, the adjoint of C_x is $C_x^\dagger: T_xM\to\mathfrak{g}$, that is, $C^\dagger\in\Omega^1(M)\otimes\mathfrak{g}$. If G acts on M freely, then C_x is injective and $(C^\dagger C)_x$ is invertible for all $x\in M$. The projection $M\to\bar{M} = M/G$ is a principal G-bundle. It has a connection such that the horizontal subspace is the orthogonal compliment of the G-orbits. The connection 1-form is $\Theta = (C^\dagger C)^{-1}C^\dagger$, whereas the curvature is $\Phi = (C^\dagger C)^{-1}\mathrm{d}C^\dagger$ on horizontal vectors.

Let ω be an equivariant form on M. Suppose G acts on M freely, then ω descends to a form ω on $\bar{M}$. We look for a gauge-invariant, supersymmetric quantity $\Upsilon(X,A)$ such that

$$\begin{aligned}&\frac{1}{\mathrm{vol}(\mathcal{G})}\int[\mathrm{d}X][\mathrm{d}A]\mathcal{O}_\omega(X,A)\Upsilon(X,A)\\ &\quad = \int[\mathrm{d}\bar{X}]\mathcal{O}_{\bar{\omega}}(\bar{X})\end{aligned} \qquad [30]$$

Mathematically, Υ corresponds to a closed equivariant form v on M such that

$$\frac{1}{\mathrm{vol}(G)}\int_{\phi\in\mathfrak{g}}[\mathrm{d}\phi]\int_M\omega(\phi)\wedge v(\phi) = \int_{\bar{M}}\bar{\omega}$$

which is [30] in the Wess–Zumino gauge. In fact, v is distribution valued in the sense of Kumar and Vergne (1993) and can be understood as an equivariant homology cycle, as in Austin and Braam (1995).

Let P be a G-bundle over $\mathbb{R}^{0|1}$ with a connection and let $\mathrm{Ad}\,P = P\times_G\mathfrak{g}\to\mathbb{R}^{0|1}$ be the adjoint bundle. Consider a (bosonic) superfield $\Lambda\in\Gamma(\mathrm{Ad}P)$. Set $\lambda = \Lambda|_{\theta=0}$ (bosonic) and $\eta = -\sqrt{-1}\mathcal{D}\Lambda|_{\theta=0}$ (fermionic). Choosing a trivialization of P, λ and η are both in $\mathfrak{g}$. Under $\theta\mapsto\theta+\epsilon$, they transform as

$$\begin{aligned}\delta\lambda &= \sqrt{-1}\epsilon(\eta + [c,\lambda])\\ \delta\eta &= \epsilon([\phi,\lambda] - \sqrt{-1}[c,\eta])\end{aligned} \qquad [31]$$

The superspace action

$$S_{\mathrm{CMR}}[X,\Lambda,A] = \sqrt{-1}\int_{\mathbb{R}^{0|1}}\mathrm{d}\theta(\Lambda, C^\dagger\mathcal{D}X)$$

is invariant under [25], [26], and [31] and, under the Wess–Zumino gauge, it is

$$\begin{aligned}&S_{\mathrm{CMR}}[x,\psi,\phi,\eta,\lambda]\\ &\quad = -\sqrt{-1}(\eta, C^\dagger\psi) - \sqrt{-1}(\lambda,\mathrm{d}C^\dagger(\psi,\psi))\\ &\quad\quad + (\lambda, C^\dagger C\phi)\end{aligned} \qquad [32]$$

If G acts on M freely, then

$$\Upsilon(X, A) = \int [\mathrm{d}\Lambda] \mathrm{e}^{-S_{\mathrm{CMR}}[X,\Lambda,A]} \qquad [33]$$

satisfies [30]. The factor $\Upsilon(X, A)$ in [30] is called "projection" in Cordes *et al.* (1996).

Let $E \to M$ be a G-equivariant vector bundle with a fixed G-invariant connection ∇, moment μ, and an invariant section s. Consider the superspace action

$$S_{\mathrm{AJ}}[X, \Xi, \Lambda, A] = S_{\mathrm{MQ}}[X, \Xi, A] + S_{\mathrm{CMR}}[X, \Lambda, A]$$

In the Wess–Zumino gauge and after the Gaussian integral over f, it becomes the Atiyah–Jeffrey action

$$\begin{aligned} S_{\mathrm{AJ}}&[x, \psi, \phi, \chi, \eta, \lambda] \\ &= S_{\mathrm{MQ}}[x, \psi, \phi, \chi] + S_{\mathrm{CMR}}[x, \psi, \phi, \eta, \lambda] \end{aligned} \qquad [34]$$

If s intersect the zero section transversely and G acts on $s^{-1}(0)$ freely, then $s^{-1}(0)/G$ is smooth and

$$\begin{aligned} \int_{s^{-1}(0)/G} \bar{\omega} = \int & [\mathrm{d}x][\mathrm{d}\psi][\mathrm{d}\phi][\mathrm{d}\chi][\mathrm{d}\eta][\mathrm{d}\lambda] \\ & \times \mathcal{O}_{\omega}(x, \psi, \phi) \mathrm{e}^{-S_{\mathrm{AJ}}[x,\phi,\phi,\chi,\eta,\lambda]} \end{aligned} \qquad [35]$$

for any closed equivariant form ω on M. Equation [35] is the formula of Atiyah and Jeffrey (1990) and of Witten (1988a) in an infinite-dimensional setting. When $s^{-1}(0)/G$ is not smooth, the right-hand side of [35] can be regarded as a definition of the left-hand side.

It is often convenient to add to S_{AJ} another term

$$\begin{aligned} \Delta S[X, \Lambda, A] &= -\frac{1}{4} \int_{\mathbb{R}^{0|1}} ([\iota_D^2 F, \Lambda], \mathcal{D}\Lambda) \\ &= \frac{\sqrt{-1}}{2} (\phi, [\eta, \eta]) + \frac{1}{2} ([\phi, \lambda], [\phi, \lambda]) \end{aligned} \qquad [36]$$

Since [36] is δ-exact and no new field is added, the integral [35] does not change if ΔS is added to S_{AJ}.

Applications to Cohomological Field Theories

We now apply the Mathai–Quillen construction formally to a number of cases in which both the rank of the vector bundle and the dimension of the base space are infinite. Thus, the (bosonic and fermionic) integrals in [24] or [35] become path integrals in quantum mechanics or quantum field theory.

Supersymmetric Quantum Mechanics

Let (M, g) be a Riemannian manifold and $LM = \mathrm{Map}(S^1, M)$, the loop space. At each point $u \in LM$, which is a map $u: S^1 \to M$, the tangent space is $T_u LM = \Gamma(u^* TM)$. In particular, $\dot{u} = \mathrm{d}u/\mathrm{d}t$, where t is a parameter on S^1, is a tangent vector at u and $u \mapsto \dot{u}$ is a vector field on LM. For any Morse function h on M, $s(u) = \dot{u} + (\mathrm{grad}\, h) \circ u$ is another vector field on LM.

Vector fields on LM can be identified as sections of the bundle $\mathrm{ev}^* TM \to S^1 \times LM$, where $\mathrm{ev}: S^1 \times LM \to M$ is the evaluation map. The Levi-Civita connection ∇ on TM pulls back to a connection on $\mathrm{ev}^* TM$ and the covariant derivatives along LM define a natural connection ∇^{LM} on $T(LM)$. For example, for any tangent vector $V \in T_u LM = \Gamma(u^* TM)$, we have $\nabla_V^{LM} s(u) = \nabla_t^u V + (\nabla_V \mathrm{grad}\, h) \circ u$, where ∇^u is the pullback connection on $u^* TM$. The Riemann curvature tensor R on M determines that on LM.

The (infinite-dimensional) analog of [22] is

$$\int [\mathrm{d}u][\mathrm{d}\psi][\mathrm{d}\chi] \exp\left(- \int_{S^1} \mathrm{d}t\, L[u, \psi, \chi] \right) \qquad [37]$$

where $\psi, \chi \in T_u LM = \Gamma(u^* TM)$ are fermionic and

$$\begin{aligned} L[u, \psi, \chi] = & \tfrac{1}{2} g(\dot{u} + \mathrm{grad}\, h, \dot{u} + \mathrm{grad}\, h) \\ & - \sqrt{-1} g(\chi, \nabla_t^u \psi + \nabla_\psi \mathrm{grad}\, h) \\ & - \tfrac{1}{4} g(\chi, R(\psi, \psi)\chi) \end{aligned} \qquad [38]$$

Here and below, factors of $\sqrt{-1}$ and 2π in [22] are absorbed in the path-integral measure. [38] is, up to a total derivative, the Lagrangian of the Euclidean $N = 2$ supersymmetric quantum mechanics on M. The partition function [37] is equal to Euler characteristic number of LM or M, which can be confirmed by an (exact) stationary-phase calculation.

Topological Sigma Model

Let Σ be a Riemann surface with complex structure ε and let (M, ω) be a symplectic manifold with a compatible almost-complex structure J. Let $\mathcal{E}$ be a vector bundle over $\mathrm{Map}(\Sigma, M)$ so that the fiber over u is $\mathcal{E}_u = \Gamma(u^* TM \times T^* \Sigma)$. For any $u \in \mathrm{Map}(\Sigma, M)$, $\mathrm{d}u \in \mathcal{E}_u$ and $u \mapsto \mathrm{d}u$ is a section of $\mathcal{E}$. The pullback of the Levi-Civita connection on TM, tensored with a connection on $T^*\Sigma$, defines a connection on $\mathcal{E}$.

The vector bundle to which we apply the Mathai–Quillen formalism is the antiholomorphic part $\mathcal{E}^{01}$ of $\mathcal{E}$. The fiber over $u \in \mathrm{Map}(\Sigma, M)$ is $\mathcal{E}_u^{01} = \Gamma((u^* TM \otimes T^*\Sigma)^{01})$. The sub-bundle $\mathcal{E}^{01}$ has a connection ∇^{01} via projection from $\mathcal{E}$. $\mathcal{E}^{01}$ has a natural section $s: u \mapsto \partial_J u = (1/2)(\mathrm{d}u + J \circ \mathrm{d}u \circ \varepsilon)$. Solutions to the equation $\bar{\partial}_J u = 0$ are pseudoholomorphic (or J-holomorphic) curves; let $\mathcal{M} = s^{-1}(0)$ be the space of such curves. Its (virtual) dimension is

$$\dim \mathcal{M} = \tfrac{1}{2} \chi(\Sigma) \dim M + 2c_1(u^* TM) \qquad [39]$$

Along any $V \in T_u\mathrm{Map}(\Sigma, M) = \Gamma(u^*TM)$, the covariant derivative of $s = \bar{\partial}_J$ is calculated in Wu (1995):

$$\nabla_V^{01}(\bar{\partial}_J) = \tfrac{1}{2}(\nabla^u V + J \circ \nabla^u V \circ \varepsilon) + \tfrac{1}{4}\nabla_V J \circ (\mathrm{d}u \circ \varepsilon + J \circ \mathrm{d}u) \qquad [40]$$

where ∇^u is the pullback connection on u^*TM.

To write the Mathai–Quillen formalism for the bundle $\mathcal{E}^{01} \to \mathrm{Map}(\Sigma, M)$, we let $\psi \in \Gamma(u^*TM)$ and $\chi \in \Gamma((u^*TM \otimes T^*\Sigma)^{01})$ be fermionic fields. Equation [23] becomes the Lagrangian

$$\begin{aligned} L[u, \psi, \chi] &= \tfrac{1}{2}\|\mathrm{d}u\|^2 + \tfrac{1}{2}(\mathrm{d}u, J \circ \mathrm{d}u \circ \varepsilon) \\ &\quad - \sqrt{-1}(\chi, \nabla^u\psi + (\nabla_\psi J) \circ \mathrm{d}u \circ \varepsilon) \\ &\quad - \tfrac{1}{8}(\chi, (R(\psi, \psi) - \tfrac{1}{2}(\nabla_\psi J)^2)\chi) \end{aligned} \qquad [41]$$

It is precisely the Lagrangian of the topological sigma model of Witten (1988b). Here, the pairing $(\cdot\,,\cdot)$ is induced by the Riemannian metric $\omega(\cdot\,, J\,\cdot)$ on M and a metric on Σ that is compatible with ε. The second term in [41], integrated over Σ, is equal to $\int_\Sigma u^*\omega = \langle[\omega], u_*[\Sigma]\rangle$.

For any differential form $\alpha \in \Omega^p(M)$, let $\mathcal{O}_\alpha(u, \psi)$ be the observable obtained from $\mathrm{ev}^*\alpha \in \Omega^p(\Sigma \times \mathrm{Map}(\Sigma, M))$ by identifying $\Omega^*(\mathrm{Map}(\Sigma, M))$ with $C(\mathrm{Map}(\mathbb{R}^{0|1}, \mathrm{Map}(\Sigma, M)))$. If α is closed and $\gamma \in H_q(\Sigma)$ is a homology cycle, then $W_{\alpha,\gamma}(u, \psi) = \int_\gamma \mathcal{O}_\alpha(u, \psi)$ is identified with a closed $(p - q)$-form on $\mathrm{Map}(\Sigma, M)$. For closed $\alpha_i \in \Omega^{p_i}(M)$ and $\gamma_i \in H_{q_i}(\Sigma)(1 \le i \le r)$, the expectation values

$$\left\langle \prod_{i=1}^r W_{\alpha_i,\gamma_i} \right\rangle = \int [\mathrm{d}u][\mathrm{d}\psi][\mathrm{d}\chi] \prod_{i=1}^r W_{\alpha_i,\gamma_i}(u, \psi)\mathrm{e}^{-S[u,\psi,\chi]} \qquad [42]$$

are the Gromov–Witten invariants of (M, ω). Moreover, [42] is nonzero only if $\sum_{i=1}^r (p_i - q_i) = \dim \mathcal{M}$.

Topological Gauge Theory

Let M be a compact, oriented 4-manifold, G, a compact, semisimple Lie group, and $P \to M$, a principal G-bundle. Denote by $\mathcal{A}$ the space of connections on P and $\mathcal{G}$, the group of gauge transformations. The Lie algebra of $\mathcal{G}$ is $\mathrm{Lie}(\mathcal{G}) = \Gamma(\mathrm{ad}\, P) = \Omega^0(M, \mathrm{ad}\, P)$. At $A \in \mathcal{A}$, the tangent space is $T_A\mathcal{A} = \Omega^1(M, \mathrm{ad}\, P)$. Both spaces have inner products if we choose an invariant inner product $(\cdot\,,\cdot)$ on the Lie algebra $\mathfrak{g}$ of G and a Riemannian metric g on M. The infinitesimal action of $\mathcal{G}$ on $\mathcal{A}$ is $C = \nabla_A$: $\mathrm{Lie}(\mathcal{G}) \to T_A\mathcal{A}$.

With a Riemannian metric, any 2-form on M decomposes into self-dual and anti-self-dual parts: $\Omega^2(M) = \Omega^2_+(M) \oplus \Omega^2_-(M)$. We consider a trivial vector bundle $\mathcal{E} \to \mathcal{A}$ whose fiber is $\Omega^2_+(M, \mathrm{ad}\, P)$. $\mathcal{G}$ acts on $\mathcal{E}$ and the bundle is $\mathcal{G}$-equivariant. The trivial connection on $\mathcal{E}$ is $\mathcal{G}$-invariant; the moment is given by $\phi \in \Gamma(\mathrm{ad}\, P) : \chi \in \Omega^2_+(M, \mathrm{ad}\, P) \mapsto [\phi, \chi]$. The bundle $\mathcal{E}$ has a natural section $s : A \in \mathcal{A} \mapsto F_A^+$, the self-dual part of the curvature. Its derivative along $V \in \Omega^1(M, \mathrm{ad}\, P) = T_A\mathcal{A}$ is $L_V s = (\nabla_A V)^+$. The section s is $\mathcal{G}$-invariant, the zero set $s^{-1}(0)$ is the space of anti-self-dual connections, and the quotient $\mathcal{M} = s^{-1}(0)/\mathcal{G}$ is the instanton moduli space. Its (virtual) dimension is

$$\dim \mathcal{M} = 4\check{h}(\mathfrak{g})k(P) - \tfrac{1}{2}\dim G(\chi(M) + \sigma(M))$$

where $\check{h}(\mathfrak{g})$ is the dual Coxeter number of $\mathfrak{g}$ and

$$k(P) = -\frac{1}{4\check{h}(\mathfrak{g})}\langle p_1(\mathrm{Ad}P), [M]\rangle \in \mathbb{Z}$$

is the instanton number of P.

We proceed with the Mathai–Quillen interpretation of Atiyah and Jeffrey (1990). Let $\psi \in \Omega^1(M, \mathrm{ad}\, P)$, $\chi \in \Omega^2_+(M, \mathrm{ad}\, P)$, $\eta \in \Gamma(\mathrm{ad}\, P)$ be fermionic fields and $\phi, \lambda \in \Gamma(\mathrm{ad}\, P)$, bosonic fields. The combination of [34] and [36] is given by the Lagrangian

$$\begin{aligned} L[A, \psi, \phi, \chi, \eta, \lambda] &= \frac{1}{2}\|F_A^+\|^2 + (\phi, \nabla_A^\dagger \nabla_A \lambda) \\ &\quad - \sqrt{-1}(\eta, \nabla_A\psi) - \sqrt{-1}(\chi, \nabla_A\psi) \\ &\quad - \sqrt{-1}(\lambda, [\psi, \psi]) \\ &\quad + \frac{\sqrt{-1}}{2}(\phi, [\chi, \chi] + [\eta, \eta]) - \frac{1}{2}\|[\phi, \lambda]\|^2 \end{aligned} \qquad [43]$$

Here, $(\cdot\,,\cdot)$ is the pairing induced by a Riemannian metric on M and an invariant inner product on $\mathfrak{g}$. With an additional topological term proportional to $(F_A, \wedge F_A)$, [43] is the Lagrangian of topological gauge theory of Witten (1988a).

There is a tautological connection on the G-bundle $\mathcal{A} \times P \to \mathcal{A} \times M$. It is invariant under the $\mathcal{G}$-action. Identifying $\Omega^*(\mathcal{A})$ with $C(\mathrm{Map}(\mathbb{R}^{0|1}, \mathcal{A}))$ and using the Cartan model, the $\mathcal{G}$-equivariant curvature is $\mathcal{F} = F_A + \sqrt{-1}\psi + \phi$. For any homology cycle $\gamma \in H_q(M)$,

$$W_\gamma(A, \psi, \phi) = \frac{1}{4\check{h}(\mathfrak{g})}\int_\gamma (\mathcal{F}, \wedge\mathcal{F}) \qquad [44]$$

corresponds to a closed $\mathcal{G}$-equivariant form on $\mathcal{A}$. For $\gamma_i \in H_{q_i}(M)(1 \le i \le r)$, the expectation values

$$\left\langle \prod_{i=1}^r W_{\gamma_i} \right\rangle = \frac{1}{\mathrm{vol}(\mathcal{G})}\int [\mathrm{d}A][\mathrm{d}\psi][\mathrm{d}\phi][\mathrm{d}\chi][\mathrm{d}\eta][\mathrm{d}\lambda] \times \prod_{i=1}^r W_{\gamma_i}(A, \psi, \phi)\mathrm{e}^{-S[A,\psi,\phi,\chi,\eta,\lambda]} \qquad [45]$$

are, up to a factor of $|Z(G)|$, Donaldson invariants of M. Moreover, [45] is nonzero only if $\sum_{i=1}^{r}(4 - q_i) = \dim \mathcal{M}$.

Other cohomological field theories can also be understood or constructed by the Mathai–Quillen formalism. Of such we mention only the topological field theories of abelian and nonabelian monopoles in Labastida and Mariño (1995), which are related to the Seiberg–Witten invariants.

See also: Characteristic Classes; Donaldson–Witten Theory; Equivariant Cohomology and the Cartan Model; *K*-Theory; Topological Quantum Field Theory: Overview; Topological Sigma Models.

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Mathematical Knot Theory

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Fundamental Concepts of the Topological Theory of Knots and Links

The first known discovery relating to knots as mathematical objects was made by Gauss around 1833 in a note that refers to the knotting together of closed curves. This investigation originated in his work on electromagnetic theory that led him to compute inductance in a system of two linked circular wires. In this note he had given an analytic formula for the linking number of a pair of knotted curves. This number is a combinatorial topological invariant (it is an integer number). Moreover, one can now show that this number is invariant under Reidemeister moves (discussed in a later section). The linking coefficient can be generalized for the case of p- and q-dimensional manifolds in $\boldsymbol{R}^{p+q+1}$. The formula for the parametrized curves $\gamma_1(t)$ and $\gamma_2(t)$ with radius vectors $r_1(t)$, $r_2(t)$ is given by the following formula:

$$\mathrm{lk}(\gamma_1, \gamma_2) = \frac{1}{4\pi} \int_{\gamma 1} \int_{\gamma 2} \frac{(r_1 - r_2, \mathrm{d}r_1, \mathrm{d}r_2)^3}{|r_1 - r_2|} \qquad [1]$$

The linking coefficient allows us to distinguish some two component links. Another approach to the link coefficient is that involving Seifert surfaces. (On this subject, see the section "Isotopies, Reidemeister moves, torus knots, and the linking number.")

A systematic study of knots in $\boldsymbol{R}^3$, however, was only begun in the second half of the nineteenth century by Tait and his followers. They were motivated by Kelvin's theory of atoms modeled on knotted vortex tubes of ether. It was expected that physical and chemical properties of various atoms could be expressed in terms of properties of knots such as the knot invariants. Even though Kelvin's theory did not work, the theory of knots grew as a subfield of combinatorial and algebraic topology. Recently, new invariants of knots have been discovered and they have led to the solution of long-standing problems in knot theory. Surprising connections between the theory of knots and statistical mechanics, quantum groups, and quantum field theory are emerging. Moreover, knot theory has been shown to be intimately connected with many problems in physics, chemistry, and biology.

Tait classified the knots in terms of the crossing number of a regular projection. A regular projection of a knot on a plane is an orthogonal projection of

the knot such that, at any crossing in the projection, exactly two strands intersect transversely. He made a number of observations about some general properties of knots which have come to be known as the "Tait conjectures." In its simplest form, the classification problem for knots can be stated as follows. Given a projection of a knot, is it possible to decide in finitely many steps if it is equivalent to an unknot. This question was answered affirmatively by W Haken in 1961. (For details, see Burde and Zieschang (1985)).

General Notions and Definitions

Let M be a closed orientable 3-manifold. A smooth embedding of S^1 in M is called a knot in M. A link in M is a finite collection of disjoint knots. The number of disjoint knots in a link is called the number of components of the link. Thus, a knot can be considered as a link with one component. Two links L, L' in M are said to be equivalent if there exists a smooth orientation-preserving automorphism $f: M \to M$ such that $f(L) = L'$. For links with two or more components, we require f to preserve a fixed given ordering of the components. Such a function f is called an ambient isotopy and L and L' are called ambient isotopic. Here, we shall take M to be $S^3 \cong \boldsymbol{R}^3 \cup \{\infty\}$ and simply write "a link" instead of "a link in S^3." The diagrams of links are drawn as links in $\boldsymbol{R}^3$. A link diagram of L is a plane projection with crossings marked as over or under. The simplest combinatorial invariant of a knot K is the crossing number $c(K)$. It is defined as the minimum number of crossings in any projection of the knot K. The classification of knots up to crossing number 17 is now known. The crossing numbers of some special families of knots are known; however, the question of finding the crossing number of an arbitrary knot is still unanswered. Another combinatorial invariant of a knot K that is easy to define is the unknotting number $u(K)$. It is defined as the minimum number of crossing changes in any projection of the knot K which makes it into a projection of the unknot. Upper and lower bounds for $u(K)$ are known for any knot K. An explicit formula for $u(K)$ for a family of knots called torus knots, conjectured by Milnor nearly 40 years ago, has been proved recently by a number of different methods. The 3-manifold $S^3 \backslash K$ is called the knot complement of K. The fundamental group $\pi_1(S^3 \backslash K)$ of the knot complement is an invariant of the knot K. It is called the fundamental group of the knot and is denoted by $\pi_1(K)$. Equivalent knots have homeomorphic complements and conversely. However, this result does not extend to links. (For details and a proof, see Manturov (2004), chapter 4).

The Fundamental Group of Knots and Its Role in Topology

For a better understanding of the above considerations, we need to introduce briefly the important concept of fundamental group in topology. The fundamental group plays an essential role in topology; it is involved in the entire technical apparatus of the subject, and likewise in all applications of topological methods. In fact, for low-dimensional manifolds (i.e., of dimension 2 or 3) the fundamental group underlies all nontrivial topological facts.

Classical knot theory is concerned with the space $S^3 \backslash K = M$, an open 3-manifold. There is a natural embedding of the torus T^2 in M, namely as the boundary of small tubular neighborhood of the knot K. Similarly, for a link we obtain a disjoint union of 2-tori in M. The principal topological invariant of a knot K is the fundamental group $\pi_1(M)$ of the complement M of K, with distinguished subgroup the natural image of $\pi_1(T^2), T \in M^2$, with the obvious standard basis. The classical theorem of Papakyriakopoulos of the 1950s asserts that a knot is equivalent to the trivial one if and only if $\pi_1(M)$ is abelian. It was known by Haken in the early 1960s that there is an algorithm for deciding whether or not any knot is equivalent to the trivial knot. However, while it appears to have been established (by Waldhausen and others in the 1960s and 1970s) that two knots are topologically equivalent if and only if the corresponding fundamental groups with labeled abelian subgroups are isomorphic, the existence of an appropriate algorithm for deciding such equivalence remains an open question. The complexity of the knot group $\pi_1(M)$ has led to the search for more effectively computable invariants to distinguish knots and links. (On this subject, see the section "Polynomial invariants of knots and links.")

Starting with the oriented diagram of the knot or link K on the plane, one calculates in the standard manner (see Crowell and Fox (1963) and Neuwirth (1965)) a presentation of the group $\pi_1(M)$ of the knot ($M = S^3 \backslash K$), obtaining one generator for the edge of the diagram of a trefoil knot and a pair of relations for each crossing. Since one relation of each such pair simply equates the pair of generators corresponding to the edges forming the upper branch of the crossing, the presentation reduces immediately to the standard one involving the same number of generators and relations. The 2-complex

L with exactly one 0-cell, and with 1-cells labeled by generators and 2-cells labeled by the relations, is then a deformation retract of M. Lifting to the universal cover we obtain a boundary operator on a complex of free $\mathbf{Z}[\pi_1]$-modules, which takes the form of a square matrix with entries from this group ring, and it is this matrix that is related to some differentiation as follows. Denoting the generators by a_i and relators by r_j, one defines the operator ∂_{ai} by

$$\partial_{a_i}(a_j) = \delta_{ij}$$
$$\partial_{a_i}(bc) = \partial_{a_i}(b) + b\partial_{a_i}(c)$$

the matrix in question then has entries q_{ij} given by

$$q_{ij} = \partial_{a_i}(r_j)$$

Mapping each generator a_i to t, we obtain a complex of modules over the ring of integer Laurent polynomials, with boundary operator the corresponding square matrix now with Laurent polynomials as entries. The determinant of this matrix turns out to be zero, and the highest common factor of its cofactors, after multiplication by a suitable power of t, turns out to be just the Alexander polynomials $A(t)$.

Let us say a bit more using a little different notation on this question. Let $A_q(K)$ and $J_q(K)$ be the Alexander polynomial and the Jones polynomial, respectively. One of the earliest problems in knot theory was: to what extent does the topological type $\mathbf{X}$ of the complementary space $X = S^3 \setminus K$ and/or the isomorphism class $\mathbf{G}$ of its fundamental group $G(K) = \pi_1(X, x_0)$ suffice to classify knots? The trefoil knot is the simplest example of nontrivial knot, so it seems remarkable that, not long after the discovery of the fundamental group of a topological space, Max Dehn (1914) succeeded in proving that the trefoil knot and its mirror image had isomorphic groups, but their knot types were distinct. Dehn's (ingenious) proof was the beginning of a long story, with many contributions which reduced repeatedly the number of distinct knot types that could have homeomorphic complements and/or isomorphic groups, until it was finally proved, quite recently, that (1) $\mathbf{X}$ determines K and (2) if K is prime, then $\mathbf{G}$ determines K up to unoriented equivalence. Thus, there are at most four distinct oriented prime knot types which have the same knot group.

The knot group $\mathbf{G}$ is finitely presented; however, it is infinite, torsion-free, and (if K is not the unknot) nonabelian. Its isomorphism class is in general not easily understood via a direct attack on the problem. In such circumstances, the obvious thing to do is to pass to the abelianized group, but unfortunately $G/[G,G] \cong H_1(X;\mathbf{Z})$ is infinite cyclic for all knots, so it is of no use in distinguishing knots. Passing to the covering space X that belongs to $[G,G]$, we note that there is a natural action of the cyclic group $G/[G,G]$ on $^{\sim}X$ via covering translations. The action makes the homology group $H_1(^{\sim}X;\mathbf{Z})$ into a $\mathbf{Z}[q,q^{-1}]$-module, where q is the generator of $G/[G,G]$. This module turns out to be finitely generated. It is the famous Alexander module. While the ring $\mathbf{Z}[q,q^{-1}]$ is not a principal ideal domain (PID), relevant aspects of the theory of modules over a PID apply to $H_1(^{\sim}X;\mathbf{Z})$. In particular, it splits as a direct sum of cyclic module, the first nontrivial one being $\mathbf{Z}[q,q^{-1}]/A_q(K)$. Thus, $A_q(K)$ is the generator of the "order ideal," and the smallest nontrivial torsion coefficient in the module $H_1(^{\sim}X)$. In particular, $A_q(K)$ is very clearly an invariant of the knot group.

We remark that when a knot is replaced by its mirror image (i.e., the orientation on S^3 is reversed), the Alexander and Jones polynomials $A_q(K)$ and $J_q(K)$ go over to $A_{q^{-1}}(K)$ and $J_{q^{-1}}(K)$, respectively. As noted earlier, $A_q(K)$ is invariant under such a change, but from the simplest example, the trefoil knot, we see that $J_q(K)$ is not. Now recall that $\mathbf{G}$ does not change under changes in the orientation of S^3. This simple argument shows that $J_q(K)$ cannot be a group invariant! Thus, it seems interesting indeed to ask about the underlying topology behind the Jones polynomial.

Isotopies, Reidemeister Moves, Torus Knots, and the Linking Number

Because each knot is a smooth embedding of S^1 in $\mathbf{R}^3$, it can be arbitrarily closely approximated by an embedding of a closed broken line in $\mathbf{R}^3$. Here we mean a good approximation such that after a very small smoothing (in the neighborhood of all vertices) we obtain a knot from the same isotopy class. However, generally this might not be the case.

Definition 1 An embedding of a disjoint union of n closed broken lines in R^3 is called a polygonal n-component link. A polygonal knot is a polygonal one-component link.

Definition 2 A link is called tame if it is isotopic to a polygonal link and wild otherwise.

All C^1-smooth knots are tame. In the sequel, all knots are taken to be smooth, hence, tame.

Definition 3 Two polygonal links are isotopic if one of them can be transformed to the other by means of an iterated sequence of elementary isotopies and reverse transformations. The

elementary isotopy, generally, is assumed to be a replacement of an edge with two edges provided that the triangle has no intersection points with other edges of the link.

It can be proved that the isotopy of smooth links corresponds to that of polygonal links; the proof is technically complicated. Like smooth links, polygonal links admit planar diagrams with overcrossings and undercrossings, having such a diagram one can restore the link up to isotopy.

Definition 4 By a planar isotopy of a smooth-link planar diagram we mean a diffeomorphism of the plane onto itself not changing the combinatorial structure of the diagram.

Obviously, planar isotopy is an isotopy, that is, it does not change the link isotopy type in $\boldsymbol{R}^3$.

Theorem 1 (Reidemeister) *Two diagrams D_1 and D_2 of smooth links generate isotopic links if and only if D_1 can be transformed into D_2 by using a finite sequence of planar isotopy and the three Reidemeister moves $\boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2, \boldsymbol{\Omega}_3$.*

Theorem 2 *Suppose that D and D' are regular diagrams of two knots (or links) K and K', respectively. Then $K \approx K' \Leftrightarrow D \approx D'$.*

We may conclude from the above theorems that the problem of equivalence of knots, in essence, is just a problem of the equivalence of regular diagrams. Therefore, a knot (or link) invariant may be thought of as a quantity that remains unchanged when we apply any one of the Reidemeister moves to a regular diagram.

Knots and links embedded in $\boldsymbol{R}^3$ can be considered as curves (families of curves) in 2-surfaces, where the latter surfaces are standardly embedded in $\boldsymbol{R}^3$. In this section we shall briefly show that all knots and links can be obtained in this manner.

Consider a handle surface S_g standardly embedded in $\boldsymbol{R}^3$ and a curve (knot) K in it. We can now ask the following question: which knot isotopy classes can appear for a fixed g? First, let us note that for $g = 0$ there exists only one knot embeddable in S^2, namely the unknot. The case $g = 1$ (torus, torus knots) gives us some interesting information. Consider the torus as a Cartesian product $S^1 \times S^1$ with coordinates $\phi, \varphi \in [0, 2\pi]$, where 2π is identified with 0. In two dimensions, the torus can be illustrated as a square with opposite sides identified. Let us embed this torus standardly in $\boldsymbol{R}^3$; more precisely,

$$(\phi, \varphi) \to ((R + r\cos\varphi)\cos\phi, \\ (R + r\cos\varphi)\sin\phi, r\sin\varphi) \quad [2]$$

Here R is the outer radius of the torus, r the small radius $(r < R)$, ϕ the longitude, and φ the meridian. For the classification of torus knots we shall need the classification of isotopy classes of nonintersecting curves in T^2: obviously, two curves isotopic in T^2 are isotopic in $\boldsymbol{R}^3$. Without loss of generality, we can assume the considered closed curve to pass through the point $(0, 0) = (2\pi, 2\pi)$. It can intersect the edges of the square several times. In addition, assume all these intersections to be transverse. Let us calculate separately the algebraic number of intersections with horizontal edges and those with vertical edges. Here, passing through the right edge or through the upper edge is said to be positive; that through the left or the lower edge is negative. Thus, for each curve of such type we obtain a pair of integer numbers. So, each torus knot passes p times the longitude of the torus, and q times its meridian, where $\mathrm{GCD}(p, q) = 1$. It is easy to see that for any coprime p and q such a curve exists: one can just take the geodesic line $\{q\phi - p\varphi = 0 \pmod{2\pi}\}$. Let us denote the torus knot by $T(p, q)$. So, in order to classify torus knots, one should consider pairs of coprime numbers p, q and see which of them can be isotopic in the ambient space $\boldsymbol{R}^3$. The simplest case is when either p or q equals 1. The next simplest example of a pair of coprime numbers is $p = 3$, $q = 2$ (or $p = 2$, $q = 3$). In each of these cases we obtain the trefoil knot. Let us state the following important result.

Theorem 3 *For any coprime integers p and q, the tori (p, q) and (q, p) are isotopic.*

Proof For a proof of this theorem, see Rolfsen (1990). Note that the (p, q) torus knot in one full torus is just the (q, p) torus knot in the other one. Thus, mapping one full torus to the other one, we obtain an isotopy of (p, q) and (q, p) torus knots. This homotopy of full tori can be expressed as a continuous process in S^3. Indeed, torus knots of type (p, q) can be represented by a series of planar diagrams. Moreover, it is possible to demonstrate a way of coding a knot (link) as a (p-strand) braid closure.

Analogously to the case of torus knots, one can define torus links which are links embedded into the torus standardly embedded in $\boldsymbol{R}^3$. We know the construction of torus knots. So, in order to draw a torus link, one should take a torus knot $K \supset T$ (one can assume that it is represented by a straight linear curve defined by the equation $q\phi - p\varphi = 0 \pmod{2\pi}$ and add to the torus T some closed nonintersecting simple curves; each curve should be nonintersecting and should not intersect K. Thus, these curves should be embedded in $T \backslash K$, that is, in the open

cylinder. Each curve on the cylinder is either contractible or passes the longitude of the cylinder once. So, each curve in $T\backslash K$ is either contractible inside $T\backslash K$, or "parallel" to K inside T, that is, isotopic to the curve given by the equation $q\phi - p\varphi = \varepsilon \,(\mathrm{mod}\, 2\pi)$ inside $T\backslash K$. Thus, the following theorem holds.

Theorem 4 *Each torus knot is isotopic to the disconnected sum of a trivial link and a link that is represented by a set of parallel torus knots of the same type* (p, q).

As we already know, a link invariant is a function defined on links that is invariant under isotopies. We shall represent links by using their planar diagrams. According to the Reidemeister theorem, in order to prove the invariance of some function on links, it is sufficient to check this invariance under the three Reidemeister moves. First, let us consider the simplest integer-valued invariant of two-component links. Let L be a link consisting of two oriented components A and B and let L' be the planar diagram of L. Consider those crossings of the diagram L' where the component A goes over the component B. There are two possible types of such crossings with respect to the orientation. For each positive crossing we assign the number $(+1)$, for each negative crossing we assign the number (-1). Let us summarize these numbers along all crossings where the component A goes over the component B. Thus, we obtain some integer number and, in fact, this number is invariant under Reidemeister moves. The so-obtained link invariant is called linking coefficient.

Polynomial Invariants of Knots and Links

By changing a link diagram at one crossing we can obtain three diagrams corresponding to links L_+, L_-, and L_0 which are identical except for this crossing. In the 1920s, Alexander gave an algorithm for computing a polynomial invariant $\Delta_K(t)$ (a Laurent polynomial in t) of a knot K, called the Alexander polynomial, by using its projection on a plane. He also gave its topological interpretation as an annihilator of a certain cohomology module associated to the knot K. In the 1960s, Conway defined his polynomial invariant and gave its relation to the Alexander polynomial. This polynomial is called the Alexander–Conway polynomial. The Alexander–Conway polynomial of an oriented link L is denoted by $\nabla_L(z)$ or simply by $\nabla(z)$ when L is fixed. We denote the corresponding polynomials of L_+, L_-, and L_0 by ∇_+, ∇_-, and ∇_0, respectively. The Alexander–Conway polynomial is uniquely determined by the following axioms.

Axiom 1 Let L and L' be two oriented links which are ambient isotopic. Then

$$\nabla_{L'}(z) = \nabla_L(z) \qquad [3]$$

Axiom 2 Let S' be the standard unknotted circle embedded in S^3. It is usually referred to as the unknot and is denoted by O. Then

$$\nabla_{\mathrm{O}}(z) = 1 \qquad [4]$$

Axiom 3 The polynomial satisfies the following skein relation:

$$\nabla_+(z) - \nabla_-(z) = z\nabla_0(z) \qquad [5]$$

We note that the original Alexander polynomial Δ_L is related to the Alexander–Conway polynomial of an oriented link L by the relation

$$\Delta_L(t) = \nabla_L(t^{1/2} - t^{-1/2}) \qquad [6]$$

In the 1980s, Jones discovered his polynomial invariant $V_L(t)$, called the Jones polynomial, while studying von Neumann algebras and gave its interpretation in terms of statistical mechanics. A state model for the Jones polynomial was then given by Kauffman (1987) using his bracket polynomial. These new polynomial invariants have led to the proofs of most of the Tait conjectures. The Jones polynomial $V_K(t)$ of K is a Laurent polynomial in t, which is uniquely determined by a simple set of properties similar to the axioms for the Alexander–Conway polynomials. More generally, the Jones polynomial can be defined for any oriented link L as a Laurent polynomial in $t^{1/2}$, so that reversing the orientation of all components of L leaves V_L unchanged. In particular, V_K does not depend on the orientation of the knot K. For a fixed link, we denote the Jones polynomial simply by V. Recall that there are three standard ways to change a link diagram at a crossing point. The Jones polynomial is characterized by the following properties:

1. Let L and L' be two oriented links which are ambient isotopic. Then
$$V_{L'}(t) = V_L(t) \qquad [7]$$
2. Let O denote the unknot. Then
$$V_{\mathrm{O}}(t) = 1 \qquad [8]$$
3. The polynomial satisfies the following skein relation:
$$t^{-1}V_+ - tV_- = (t^{1/2} - t^{-1/2})V_0 \qquad [9]$$

An important property of the Jones polynomial that is not shared by the Alexander–Conway polynomial is its ability to distinguish between a knot and its mirror image. More precisely, we have the following result. Let K_m be the mirror image of the knot K. Then

$$V_{K_m}(t) = V_K(t-1) \quad [10]$$

Since the Jones polynomial is not symmetric in t and t^{-1}, it follows that in general

$$V_{K_m}(t) \neq V_K(t) \quad [11]$$

We note that a knot is called amphicheiral (achiral in biochemistry) if it is equivalent to its mirror image. We shall use the simpler biochemistry term. So, a knot that is not equivalent to its mirror image is called chiral. The condition expressed by [11] is sufficient but not necessary for chirality of a knot. The Jones polynomial did not resolve the following conjecture by Tait concerning chirality: if the crossing number of a knot is odd, then it is chiral. However, it has been demonstrated recently that a 15-crossing knot provides a counterexample to the chirality conjecture.

New Invariants and Their Applications in Mathematical Physics

There was an interval of nearly 60 years between the discovery of the Alexander polynomial and the Jones polynomial. Since then a number of polynomials and other invariants of knots and links have been found. A particularly interesting one is the two-variable polynomial generalizing V, called the HOMFLY polynomial (name formed from the initials of authors of the article (Freyd *et al.* 1985) and denoted by P. The HOMFLY polynomial $P(\alpha, z)$ satisfies the following skein relation:

$$\alpha^{-1}P_{+} - \alpha P_{-} = zP_0 \quad [12]$$

Both the Jones polynomial V and the Alexander–Conway polynomial ∇_L are special cases of the HOMFLY polynomial. The precise relations are given by the following theorem.

Theorem 5 *Let L be an oriented link. Then the polynomials P_L, V_L, and ∇_L satisfy the following relations*:

$$V_L(t) = P_L(t, t^{1/2} - t^{-1/2}) \text{ and } \nabla_L(z) = P_L(1, z) \quad [13]$$

After defining his polynomial invariant, Jones also established the relation of some knot invariants with statistical mechanical models. Since then this has become a very active area of research. By constructing a typical statistical mechanics model – the star–triangle relations of the Yang–Baxter equations are an example of such model – one obtains a state model for the Alexander or the Jones polynomial of a knot, by associating to the knot a statistical system, whose partition function

$$Z_K := \sum E_K(s)\omega(s) \quad [14]$$

gives the corresponding polynomial. (For details, see Jones (1989)). In the function above, $\omega = F(X, S) \to \mathbf{R}$ is a weight function and the sum is taken over all states $s \in F(X, S)$. The energy E_k of the system (X, S) is a functional,

$$E_k : F(X, S) \to \mathbf{R}, k \in K \quad [15]$$

where the subscript $k \in K$ indicates the dependence of energy on the set K of auxiliary parameters, such as temperature, pressure, etc.

However, these statistical models did not provide a geometrical or topological interpretation of the polynomial invariant. Such an interpretation was provided by Witten (1989) by applying ideas from quantum field theory to the Chern–Simons Lagrangian. In fact, Witten's model allows us to consider the knot and link invariants in any compact 3-manifold M.

Vassiliev Invariants and the Space of All Knots: New Generalizations of Knot Theory

An entirely new collection of knot invariants, which arose out of techniques pioneered by Arnold in singularity theory, has been introduced by V A Vassiliev in the 1990s. The knot invariants, like the Alexander polynomial, associate a knot with some sort of mathematical quantity. A Vassiliev invariant, on the other hand, is an invariant that satisfies a set of conditions. In this sense, all the invariants introduced above – the Jones polynomial, the HOMFLY and the Kauffman polynomial, the Conway polynomial, and the Alexander polynomial – can all be shown to be Vassiliev invariants. However, not all the knot invariants are Vassiliev invariants, for instance, the signature of a knot is not a Vassiliev invariant. The new Vassiliev invariants have a solid basis in a very interesting new topology, where one studies not a single knot, but a space of all knots. Vassiliev's knot invariants are rational numbers. They lie in vector space V_i of dimension d_i, $i = 1, 2, 3, \ldots$, with invariants in V_i having "order" i. These invariants are built from different families of crossing changes.

Considering that Vassiliev's invariants require introducing an important conceptual change, shifting our attention from the knot K, which is the image of S^1 under an embedding $\phi: S^1 \to S^3$, to the embedding ϕ itself. A knot type K thus becomes an equivalence class $\{\phi\}$ of embeddings of S^1 into S^3. The space of all such equivalence classes of embeddings is disconnected, with a component for each smooth knot type. In this way, one passes from embeddings to smooth maps, thereby admitting maps which have various types of singularities. Let $^{\sim}M$ be the space of all smooth maps from S^1 to S^3. This space is connected and contains all knot types. Our space will remain connected and will contain all knot types if we place two mild restrictions on our maps. Let M denote the collection of all $\phi \in {}^{\sim}M$ such that $\phi(S^1)$ passes through a fixed point α and is tangent to a fixed direction at α. The space M has some interesting properties, the main one being that it can be approximated by certain affine spaces, and these affine spaces contain representatives of all knot types. The walls between distinct chambers in M constitute the discriminant Σ, that is, $\Sigma = \{\phi \in M \mid \phi\}$ has a multiple point or a place where its derivative vanishes or other singularities. The space $M - \Sigma$ is our space of all knots.

The additive properties of the Alexander and Jones polynomials have a very attractive interpretation in terms of Vassiliev invariants. By a result of Bar-Natan, all coefficients of the Alexander polynomial are Vassiliev invariants (see Bar-Natan (1995)). The same can be said of the Jones polynomial, as proved by a theorem of Birman and Lin (1993). There is an attractive formula due to Kontsevich expressing all Vassiliev invariants analytically in terms of multiple integrals, assuming that the knot or link diagram comes with some generic Morse function (e.g., the projection of the planar diagram on the y-axis). Moreover, from the work of Kontsevich it follows that it is possible to give a purely combinatorial characterization of all Vassiliev invariants (other than the one mentioned above) by associating to an oriented knot K in R^3 (given via coordinates $z = z(t)(= x(t) + iy(t)), t)$ a chord diagram, which is just a circle with $2k$ distinct points labeled P_j, Q_j, $j = 1, 2, \ldots, k$, marked on it, and by imposing certain relations on the free abelian group freely generated by all chord diagrams.

Theorem 6 *Let $V_K(t)$ be the Jones polynomial of a knot K. Let $V_K(q)$ be the infinite series obtained from $V_K(t)$ by substituting $e^q (= 1 + q + q^2/2! + \cdots = \sum_{n=0}^{\infty} q^n/n!)$ for t. So we may write*

$$V_K(q) = b_0 + b_{1q} + b_2 q^2 + \cdots$$

Then $J_m(K) = b_m$ is a Vassiliev invariant induced by the Jones polynomial of order (at most) m.

The structure and significance of the HOMFLY and Kauffman polynomials can be interpreted in the language of Vassiliev invariants, which are invariants of finite type. The notion of finite type is of extraordinary significance in studying these invariants. One reason for this is the following basic lemma:

Lemma 7 *If a graph G (an embedded 4-valent graph) has exactly k nodes, then the value of a Vassiliev invariant v_k of type k on G, $v_k(G)$, is independent of the embedding of G.*

Let us show briefly this important result. Suppose V is any invariant of oriented links taking values in some abelian group. This V can be extended to be an invariant of singular links in the following way (Kauffman 2001): a singular link is an immersion of simple closed curves in S^3 with finitely many transverse double-points. These self-intersections are required to remain transverse in any isotopy demonstrating the equivalence of such singular links. If the definition of V has been extended over singular links with $n - 1$ double points, define it on a singular link $L_\times$ with n singularities by

$$V(L_{¥}) = V(L_+) - V(L_-)$$

where $V(L_\times)$, $V(L_+)$, and $V(L_-)$ are identical except near a point where they form a node. Note that $V(L_+)$ and $V(L_-)$ each has $n - 1$ double points. Then V is called a Vassiliev invariant of order n, or an invariant of finite type n, if $V(L) = 0$ for every L with $n + 1$ or more singularities. Recall the Alexander–Conway polynomial invariant, $\nabla_L(z) \in Z[z]$, of oriented links defined by $\nabla_{\text{unknot}}(z) = 1$ and

$$\nabla_{L_+}(z) - \nabla_{L_-}(z) = z\nabla_{L_0}(z)$$

Extend this over singular links by the above method. Then if $L_\times$ is a link with r singularities, $\nabla_{L_\times}(z) = z\nabla_{L_0}(z)$, where L_0 is a link with $r - 1$ singularities. Thus, by induction on r, if L has r singularities then $\nabla_L(z)$ has a factor of z^r. This implies at once that the coefficient of z^n in the Conway polynomial of a link is a Vassiliev invariant of order n. Now suppose one considers the HOMFLY polynomial and makes the substitution $(l, m) = (it^{N/2}, i(t^{-1/2} - t^{1/2}))$. The characterizing skein relation becomes

$$t^{N/2}P(L_+) - t^{-N/2}P(L_-) = (t^{1/2} - t^{-1/2})P(L_0)$$

Note that this becomes the Jones polynomial when $N = 2$. Now make the further substitution $t = \exp x$. Here $\exp x$ should be thought of as the classical power series expansion. Of course, $\exp(x/2)$ and

$\exp(-x/2)$ have power series expansions; the power series can be multiplied and added to give another power series. Thus, $P(L)$ has a power series expansion in powers of x. It follows immediately that $P(L_+)-P(L_-)=xS(x)$ for some power series $S(x)$. Hence, the proof used for the Conway polynomial shows at once that the coefficient of x^n in the power series expansion of $P(L)$ is a Vassiliev invariant of order n.

All present studies of Vassiliev invariants clearly indicate a major role of these invariants in the future developments of knot theory and topological quantum field theories. Many questions in knot theory remain open, nevertheless, in future it will, very likely be one of the most fruitful and beautiful subjects of research in mathematics and in mathematical physics. Knot theory also attracts attention from the fact that it is revealing new astounding and profound links between geometry, algebra, and topology.

See also: Finite-Type Invariants; The Jones Polynomial; Knot Invariants and Quantum Gravity; Knot Theory and Physics; Kontsevich Integral; String Topology: Homotopy and Geometric Perspectives; Topological Knot Theory and Macroscopic Physics; Topological Quantum Field Theory: Overview.

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Matrix Product States *see* Finitely Correlated States

Mean Curvature Flow *see* Geometric Flows and the Penrose Inequality

Mean Field Spin Glasses and Neural Networks

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Introduction and Models

Rarely has a paper with a simple title as "A solvable model of a spin glass" had such a tremendous impact on both physics and mathematics as the seminal paper of 1972 by Sherrington and Kirkpatrick, which introduced what is now known as the Sherrington–Kirkpatrick (SK) mean-field spin glass model. As solvable as it might have appeared to the authors, it was soon found that the heuristic solution, based on the so-called replica method, was physically unacceptable. The reason was a tacit assumption, now known as replica symmetry, that proved unfounded. Several years later, Giorgio Parisi provided an ingenious way out through his continuous replica symmetry-breaking scheme, that presented a solution that, through its complexity and intrinsic beauty, both stunned and fascinated the community. Unraveling the mysteries involved in this solution has presented a challenge and driving force for the last three decades of mathematical statistical mechanics, while the use of the method in theoretical physics opened the path to solving a wide variety of problems not only in the theory of disordered magnets, but also in neural networks and combinatorial optimization. In this article the focus is on the mathematical results obtained in the study of this and a number of related models.

Mean-Field Models

Mean-field models have played an important role in statistical mechanics by providing simple, solvable models in which some of the complex phenomena, such as phase transitions, could be studied and understood. For example, the Curie–Weiss model of a ferromagnet describes N spin variables σ_i (taking values ± 1) in interaction. The simplifying assumption compared to more realistic models, such as the Ising model, is to ignore the spatial structure of the model and allow all spins to interact with each other with equal strength. This yields to a Hamiltonian function of the form

$$H_N(\sigma) = -\frac{J}{N}\sum_{i,j=1}^{N}\sigma_i\sigma_j + h\sum_{i=1}^{N}\sigma_i \qquad [1]$$

where J is a coupling constant and h a magnetic field. This from of the interaction implies that the Hamiltonian is in fact just a function of the empirical magnetization $m_N(\sigma) = N^{-1}\sum_{i=1}\sigma_i$, and this allows one to use methods from the theory of large deviations to analyze rather easily the corresponding Gibbs measures

$$\mu_{\beta,N}(\sigma) \equiv \frac{e^{-\beta H_N(\sigma)}}{Z_{\beta,N}} \qquad [2]$$

The SK Model

This model was a straightforward attempt to introduce a mean-field version of models with randomly interacting spins. The interest in such models arose from the discovery of certain alloys of ferromagnets and conductors (e.g., AuFe and CuMn) that had been found to exhibit very unusual magnetic properties. Ruderman and co-workers had proposed that in these models the magnetic ions with magnetic moments S_i and S_j located at the points x_i and x_j would interact via an exchange interaction of the form

$$\frac{\cos(k_f(x_i - x_j))}{|x_i - x_j|^3} S_i \cdot S_j$$

Since the positions of the magnetic ions in the alloy are random, the signs of their interaction would be oscillatory. Anderson proposed a simplified model, in the spirit of the Ising model, where spins taking values ± 1 located on a regular lattice would interact via nearest-neighbor couplings J_{ij} modeled as i.i.d. random variables uniformly distributed on an interval $[-J, J]$. In the spirit of the Curie–Weiss model, Sherrington and Kirkpatrick then proposed the mean-field model where any two spins would interact via i.i.d. Gaussian random variables J_{ij} of mean zero and variance one. The SK Hamiltonian is thus given by

$$H_N^{\mathrm{SK}}(\sigma) \equiv -\frac{J}{\sqrt{N}}\sum_{1\le i<j\le N} J_{ij}\sigma_i\sigma_j + h\sum_{i=1}^{N}\sigma_i \qquad [3]$$

where the normalization is chosen to ensure that the variance of H_N is an extensive quantity. Although the two Hamiltonians superficially look similar, the main feature that allows one to solve the Curie–Weiss model is absent in the SK model: there is no way to write the Hamiltonian as a function of macroscopic variable(s) such as the magnetization. This implies that all methods known to solve the Curie–Weiss model fail here. The approach used systematically in the physics literature to overcome

this difficulty is to try to compute the mean free energy $f_{\beta,N} \equiv -(1/\beta N)$, $\mathbb{E}\ln Z_{\beta,N}$ using the formal identity $\ln x = \lim_{q\downarrow 0} q^{-1}(x^q - 1)$. For $q \in N$, one easily sees that (putting $h = 0$)

$$\mathbb{E}Z^q_{\beta,N} = \sum_{\sigma^1,\ldots,\sigma^q} \exp\left(\frac{\beta^2 J^2}{2} N \sum_{a,b=1}^{q} \sum_{i<j} \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b\right)$$

This expression looks already more like the partition function of an ordinary mean-field model, and the computation with standard methods seemed feasible. However, passage to the limit $q\downarrow 0$ remains a highly risky enterprise, and it took the genius of Parisi to develop an approach that provided at least a physically meaningful and convincing answer. The replica method being dealt with elsewhere in this encyclopedia, this approach is not explained any further here, although we will explain the nature of the result in the light of recent rigorous work later on.

Site Disordered Models

The difficulties encountered with the random-bond interactions led readily to proposals of mean-field models that were closer to the Curie–Weiss model – from the point of view that they allowed the Hamiltonian to be written as a function of macroscopic variables. The most important of these models was introduced by Figotin and Pastur. Here the disorder was introduced as an M-dimensional vector ξ_i for each site i. The components of this vector are usually taken as i.i.d. random variables ξ_i^μ taking values ± 1 with equal probability. One can then introduce M-dimensional vectors as macroscopic variables that generalize the magnetization with components

$$m_N^\mu(\sigma) \equiv N^{-1} \sum_{i=1}^{N} \xi_i^\mu \sigma_i$$

The Hamiltonian can then be written as

$$\begin{aligned} H_N(\sigma) &= -N \sum_{\mu=1}^{M} (m_N^\mu(\sigma))^2 \\ &= -\frac{1}{N} \sum_{i,j=1}^{N} \sigma_i \sigma_j \sum_{\mu=1}^{M} \xi_i^\mu \xi_j^\mu \end{aligned}$$

These models were indeed found to be solvable with tools similar to those used in the Curie–Weiss case; however, they proved disappointing in that the solution did not show the characteristic features expected in a spin glass. In fact, it turns out the these models behave very much like a mean-field ferromagnet, except that as they display not just two equilibrium states at low temperatures, but $2M$ of them, concentrated on spin configurations σ for which $m_N(\sigma)$ takes values close to one of the values $\pm m^*(\beta)e_\mu$, where e_μ is the μ-unit vector in $\mathbb{R}^M$ and $m^*(\beta)$ solves the equation $m = \tanh(\beta m)$ known from the Curie–Weiss model. This model might have been forgotten, had it not been rediscovered in 1982 by Hopfield in the context of neural networks. Hopfield realized that if σ_i are interpreted as the activation states ("firing" and "not firing") of neurons in the brain, the form of the interaction in this model is exactly the one proposed earlier by Hebb for synaptic interaction between neurons having "learned" the M "patterns" ξ^μ in the past. He went on to interpret $H_N(\sigma)$ as the Lyapounov function of the retrieval algorithm by which the brain would recognize the learned pattern. Naturally, the fact the the configurations ξ^μ are minima of H_N then implies the functioning of the algorithm. The important observation of Hopfield was that, based on numerical experiments, the algorithm failed when M became too large. In fact, he observed a breakdown of the memory if $M \geq 0.14N$. This meant that the interesting asymptotics in this model required to consider M as an increasing function of N. This regime was not covered by large-deviation-type results and an intensive program to investigate this model was initiated. Again, the replica method could be employed and yielded a very rich structure of the model, including an explanation of the findings of Hopfield. These models also turned out to be an important starting point for the rigorous analysis.

Gaussian Processes and Derrida's Models

While the models discussed so far were motivated from the point of view of randomly interacting spins, Derrida had the consequential idea to view the Hamiltonian of such a model simply as a random process indexed by the set of all spin configuration. In the case of the SK model, this process was, moreover, a Gaussian process and thus characterized entirely by its mean and variance. For $h = 0$ we see that

$$\mathbb{E}H_N^{\mathrm{SK}}(\sigma)H_N^{\mathrm{SK}}(\sigma') = \frac{N}{2}(r_N(\sigma,\sigma'))^2 - \frac{1}{2} r_N(\sigma,\sigma')$$

where $r_N(\sigma,\sigma') \equiv N^{-1}\sigma_i\sigma_i'$ is usually called the overlap. This opened the view to a much larger class of models. In particular, the simplest model from this perspective corresponds to taking $H_N(\sigma)$ as a process of i.i.d. random variables. Derrida called this the *random-energy* model (REM). He also noted

that it could be seen as the limit if a sequence of the so-called p-spin SK models corresponding to the covariance of the Hamiltonian being $N(r_N(\sigma,\sigma'))^p$. On the other hand, Derrida observed that another class of models could be defined that were easier to analyze while exhibiting much of the complex properties of the SK model. These are obtained by choosing the covariance not as a function of the overlap (resp. the Hamming distance), but of a ultra-metric distance related to $d_N(\sigma,\sigma') \equiv N^{-1}(\inf\{i:\sigma_i \neq \sigma_i'\} - 1)$. These models, called generalized Random-Energy Models (GREM) were analyzed by Derrida and Gardner in the 1980s and are now the only models where the full predictions of the Parisi theory can be rigorously justified. This is discussed in some detail later.

Further Models and Applications

There is a wealth of problems that can be interpreted in terms of disordered mean-field models, and which may be analyzed using methods developed here. Some of the most notable ones that have received more attention lately include: the perceptron, a feed-forward neural network was analyzed first by Gardner using the replica method. Very recently, Shcherbina and Tirozzi gave a rigorous justification of this result. The p-satisfiability problem is an important problem in computer science that also can be analyzed with the replica method. Rigorous results are still very limited. The number partitioning problem can be formulated as a random-energy model. Also, the most famous problem in combinatorial optimization, the traveling salesman problem, can be solved heuristically with the replica method. Another emerging field are applications to coding theory.

Formulation of the Problem

Given a model, that is, a Hamiltonian function defined as a random process, the ultimate goal is to describe the asymptotic properties of the corresponding Gibbs measure, ideally identifying a (random or deterministic) limiting measure, as a function of the temperature, β^{-1}, and other parameters, such as the magnetic field h.

The first steps in this direction concerns global properties:

- Does the ground-state energy density,

$$\lim_{N\uparrow\infty} \max_{\sigma\in\mathcal{S}_N} H_N(\sigma)$$

converge (in what sense?) and what is the limit?

- What is the limit of the free energy

$$f_{\beta,N} \equiv \frac{-1}{\beta N} \ln Z_{\beta,N}$$

It has been noted in the mid-1990s that such quantities are usually self-averaging, for example, in the sense that

$$\lim_{N\uparrow\infty} (f_{\beta,N} - \mathbb{E}f_{\beta,N}) = 0, \quad \text{a.s.}$$

due to the concentration of measure phenomenon. However, until very recently, the existence of the limits was considered an open problem in most of the models described above. Guerra and Toninelli (2002) discovered that a clever use of comparison inequalities for convex functions of Gaussian processes allows one to prove *a priori* the existence of limits at least in the case of models based on Gaussian processes (SK, GREM). The main task is the computation of the values of the limit.

If the free energy is known as a function of sufficiently many parameters, one can frequently compute a number of correlation functions that characterize the limiting measure as well. What one should compute is somewhat model dependent.

Geometry of Gibbs Measures and Multi-Overlap Distributions

The problem of satisfactorly describing the asymptotic geometric properties of random Gibbs measures on $\{-1,1\}$ is rendered difficult as the symmetries of the problem make the use of local topologies seem unattractive. A reasonable way of solving this problem is as follows. Let D_N be a distance on $\mathcal{S}_N$ normalized so that $\max_{\sigma,\tau\in\mathcal{S}_N} D_N(\sigma,\tau) = 1$. Then consider the mass distribution around any fixed point σ,

$$m_\sigma(x) \equiv \mu_{\beta,N}(D_N(\sigma,\sigma') \leq x)$$

and construct the biased empirical average

$$\mathcal{K}_{\beta,N} \equiv \sum_{\sigma\in\mathcal{S}_N} \mu_{\beta,N}(\sigma)\delta_{m_\sigma(\cdot)}$$

The set of distributions of these random measures is compact (with respect to the weak topology) and thus we can expect to construct limits. The law of $\mathcal{K}_{\beta,N}$ is fully determined by the family of averaged distributions of the distances between n independent copies of σ drawn from the Gibbs measures,

$$\mathbb{E}\mu_{\beta,N}^{\otimes n}(D_N(\sigma^1,\sigma^2),\ldots,D_N(\sigma^{n-1},\sigma^n))$$

In the SK models, one chooses

$$D_N(\sigma,\tau) = 1 - \frac{1}{N}\sum_i \sigma_i\tau_i$$

so that these quantities can be expressed as distributions of the overlaps $(1/N)\sum_i \sigma_i\tau_i$, between n "replica" spin variables. In the GREM models, it is natural to chose as distance the lexicographic distance used in the construction of the models. In this case, the limits of $\mathcal{K}_{\beta,N}$ can be constructed explicitly and it was shown that they can be expressed in terms of the size-biased empirical family size distribution of a certain continuous state branching process via a model-dependent time change. Since this plays a key rôle not only in the GREMs but in other models as well, we will go into some detail to elucidate this structure.

In the GREM models, it can be shown that the quantity $\mathcal{K}_{\beta,N}$ converges (weakly in law) to the corresponding $\mathcal{K}$ obtained from a time change of the family of measures θ_t, namely

$$\theta_t^{m_\beta} \equiv \theta_{\ln m(t) - \ln m(0)}$$

where m is a nondecreasing function that can be computed explicitly. Namely, if $\mathbb{E}X_\sigma X_\tau = A(\mathrm{d}_N(\sigma,\tau))$, and $\bar{a}$ denotes the right-derivative of the concave hull of A, then

$$m(x) = \min\left(\beta^{-1}\sqrt{2\ln 2}/\sqrt{\bar{a}(x)}, 1\right)$$

As explained below, similar results are expected in the SK models.

Neveu's Process and Random Genealogies

The random structure of the limiting Gibbs measures of the GREM models (and presumably also the SK models, even though this is not proven) can be traced to a continuous-state branching process introduced by Neveu, and an induced associated random genealogy on the unit interval. Let Z_t be a time-homogeneous continuous-time Markov process with state space $\mathbb{R}_+$ characterized by the Laplace transform of its transition kernel

$$\mathbb{E}(\mathrm{e}^{-\lambda Z_t} | Z_0 = a) = \exp\left(-a\lambda^{\mathrm{e}^{-t}}\right)$$

Based on this process, construct a two-parameter process $Z(t, a)$ with the property that, for any $a, b > 0$, the processes $Z(\cdot, a)$ and $Z(\cdot, a+b) - Z(\cdot, a)$ are independent and have the same laws as Z_t with initial conditions a, resp. b. It follows that $Z(t,\cdot)$ is a stable subordinator with exponent e^{-t}. Now let $\theta_t(a) \equiv Z(t,a)/Z(t,1)$, as a function on $[0,1]$, θ_t being a random probability distribution function (of pure point type). Any such family μ_t of distributions defines in a natural way a genealogical structure on $[0, 1]$. Define the ancestor of $\alpha \in [0,1]$ at time $t < 1$ to be $a_t(\alpha) \equiv \theta_t(\theta_1^{-1}(\alpha))$, where θ^{-1} is the right-continuous inverse of the nondecreasing function θ.

We say that, for $\alpha, \alpha' \in [0,1], q(\alpha,\alpha') = t$ if and only if $t = \sup(s : a_s(\alpha) = a_s(\alpha'))$. It is easy to see that $1-q$ defines an ultra-metric distance. We can associate with this the distribution size of the offspring of an ancestor at time t, $m_\alpha(t) = |\alpha' : q(\alpha,\alpha') \le t|$, and its size-biased empirical distribution

$$\mathcal{K} \equiv \int_0^1 \mathrm{d}\alpha\, \delta_{m_\alpha(\cdot)}$$

Interpolation Methods and Guerra's Integral Representation

Among the very important tools for the analysis of Gaussian models in particular have been the interpolation methods that allow one to compare functions of processes with different covariance. While these methods go back to early work on Gaussian processes (Slepian, Kahane), they have been employed with remarkable success in the present context. Mostly, they consist in introducing an interpolating Hamiltonian $H^t(\sigma) \equiv \sqrt{t}H(\sigma) + \sqrt{1-t}K(\sigma)$, where K is a reference process that has certain desired properties. Given any function F of the process (e.g., the free energy of the model), one then represents

$$F(H) = F(K) + \int_0^1 \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t} F(H^t)$$

Often the derivative on the right-hand side can be controlled rather well, for example, because of some obvious positivity properties.

Example 1 (Guerra and Toninelli). Choose

$$K(\sigma) = \frac{1}{\sqrt{M}} \sum_{i<j=1}^{M} J'_{ij}\sigma_i\sigma_j + \frac{1}{\sqrt{N-M}} \sum_{i<j=M+1}^{N} J'_{ij}\sigma_i\sigma_j$$

and consider the free energy $F(H^t) = f^t_{\beta,N}$. Then, first $F(H^0_N) = F(H_M) + F(H_{N-M})$. On the other hand,

$$\frac{\mathrm{d}}{\mathrm{d}t} F(H^t_N) = -\frac{1}{2N}\mu^t_{\beta,N}\left(\sum_{i<j=1}^{N} \frac{\sigma_i\sigma_j J_{ij}}{tN} - \sum_{i<j=1}^{M} \frac{J'_{ij}\sigma_i\sigma_j}{\sqrt{(1-t)M}} + \sum_{i<j=M+1}^{N} \frac{J'_{ij}\sigma_i\sigma_j}{\sqrt{(1-t)(N-M)}}\right)$$

A key tool to be used at this stage is the so-called Gaussian integration by parts formula, $\mathbb{E}gf(g) = \mathbb{E}f'(g)$. Applied here, this gives

$$\frac{\mathrm{d}}{\mathrm{d}t}F(H_N^t) = \frac{\beta}{4N^2}\mu_{\beta,N}^{t,\otimes 2}\left(\left(\sum_{i=1}^{N}\sigma_i\sigma_i'\right)^2 - \frac{N}{M}\left(\sum_{i=1}^{M}\sigma_i\sigma_i'\right)^2 - \frac{N}{N-M}\left(\sum_{i=M+1}^{N}\sigma_i\sigma_i'\right)^2\right) \geq 0$$

This proves superadditivity of $N\mathbb{E}f_{\beta,N}$,

$$N\mathbb{E}f_{\beta,N} \geq M\mathbb{E}f_{\beta,M} + (N-M)\mathbb{E}f_{\beta,N-M}$$

which, in turn, implies convergence of $\mathbb{E}f_{\beta,N}$ to a limit $\mathbb{E}f_\beta$. Moreover, standard concentration of measure estimates show then that $f_{\beta,N}$ also converges almost surely.

Example 2 (Guerra, Aizenman–Sims–Starr). A more complicated application of the interpolation method allows one to relate the free energy to Parisi's solution. This was first found by Guerra (2003), but a different, and in some sense more intuitive formulation, was given later by Aizenman *et al.* (2003). It is based on the following construction. We consider a centered Gaussian process $H_N(\sigma)$ on $\mathcal{S}_N$ with covariance given by $Ng(R_N(\sigma,\sigma'))$ for some even convex function $g:[-1,1] \to [0,1]$. Let us take $F(H_N) = \ln \mathbb{E}_\sigma \mathrm{e}^{\beta H_N(\sigma)}$ (the *a priori* expectation $\mathbb{E}_\sigma$ need not be symmetric, but may incorporate a magnetic field). Before using comparison, we now want to go to a larger space. For this, introduce some set $\mathcal{A}$ equipped with some positive-definite quadratic form q, normalized such that $q_{\alpha,\alpha} = 1$, and $|q_{\alpha,\alpha'}| \leq 1$, $\forall_{\alpha,\alpha' \in \mathcal{A}}$. Let $\mathbb{P}_\alpha$ denote some probability measure on $\mathcal{A}$. Now introduce a centered Gaussian process κ_α on $\mathcal{A}$, independent of H_N, whose covariance is given by $\mathbb{E}\kappa_\alpha\kappa_{\alpha'} = r(q_{\alpha,\alpha'}) \equiv q_{\alpha,\alpha'}g'(q_{\alpha,\alpha'}) - g(q_{\alpha,\alpha'})$. Define

$$G(H_N + \sqrt{N}\kappa) = \ln\left(\mathbb{E}_\sigma\mathbb{E}_\alpha\, \mathrm{e}^{-\beta(H_N(\sigma)+\sqrt{N}\kappa_\alpha)}\right)$$

Obviously, $G(H_N,\kappa) = F(H_N) + \widetilde{F}(\kappa)$, where $\widetilde{F}(\kappa) = \ln(\mathbb{E}_\alpha\, \mathrm{e}^{-\beta\sqrt{N}\kappa_\alpha})$. The amazing idea is now to compare the process $(H_N + \kappa)$ with another process $\eta_{\sigma,\alpha}$ whose covariance is a linear function of $R_N(\sigma)$ (this is in some sense a Slepian's process), and that otherwise is smaller than the covariance of $(H_N + \kappa)$; to wit

$$\mathbb{E}\eta_{\alpha,\sigma}\eta_{\alpha',\sigma'} = R_N(\sigma,\sigma')g'(q_{\alpha,\alpha'})$$

By these choices of covariances, one has that for $x \in [-1,1]$, $y \in [0,1]$, since g is even and convex,

$$g(x) + yg'(y) - g(y) \geq xg'(y)$$

It is an immediate consequence of Kahane's theorem, respectively the same interpolation argument given above, that

$$\mathbb{E}G(H_N + \kappa) \leq \mathbb{E}G(\eta)$$

which translates into

$$\mathbb{E}F(H_N) \leq \mathbb{E}G(\eta) - \mathbb{E}\widetilde{F}(\kappa)$$

It is clear that we can optimize this bound by choosing $\mathcal{A}, q$, and P_α. Of course, the difficulty would be to find such a minimum. A first simplification of this optimization problem is to consider instead of the deterministic structure of $\mathbb{P}$ and q random-probability measures on the space of probability measures and quadratic forms on $\mathcal{A}$, to average over the preceding equation with respect to their laws, and then take the infimum over all such random structures. This gives a (still incalculable) bound that Aizenman *et al.* (2003) have shown to be asymptotically sharp, that is, they showed that

$$\lim_{N\uparrow\infty}\mathbb{E}F(H_N) = \lim_{N\uparrow\infty}\inf_{\mathcal{A},\,\mu}\mathbb{E}_\mu(\mathbb{E}G(\eta) - \mathbb{E}\widetilde{F}(\kappa))$$

where μ is short for all probability measures on the space of $(\mathbb{P}_\alpha, q_{\alpha,\alpha'})$ on $\mathcal{A}$ (called "random overlap structures"(rosts) in Aizenman *et al.* (2003)). Guerra's bound consists in restricting the infimum to a class of rosts where the bound is calculable 'explicitly'. Maybe unsurprisingly, this is exactly the class of asymptotic models that have already arisen in the GREMs. In fact, we set $\mathcal{A} = [0,1]$, $\mathcal{M} \equiv \{m:[0,1] \to [0,1]$, non-decreasing$\}$, let q be the random genealogical distance associated to the family of measures θ_t^m, and let $\mathbb{P}_\alpha$ be the probability measure on $\mathcal{A}$ whose distribution function is $\theta_1^m(\alpha)$. Then Guerra's bound states that

$$\lim_{N\uparrow\infty}\mathbb{E}F(H_N) \leq \lim_{N\uparrow\infty}\inf_{m\in\mathcal{M}}\mathbb{E}G(\eta) - \mathbb{E}\widetilde{F}(\kappa)$$

where the expectations relate to all random quantities involved. By self-averaging, the same result holds almost surely. The right-hand side of this equation is known as (a particular formulation of) the famous Parisi solution. In fact, define the function $f(q,y)$ as the solution of the nonlinear partial differential equation

$$\partial_q f + \frac{1}{2}\left(\partial_y^2 f + m(q)(\partial_y f)^2\right) = 0$$

with final conditions

$$f(1,q) = \ln\cosh\beta y$$

These equations can be solved by elementary means in the case when m is a step function. It turns out that, for given m,

$$\mathbb{E}G(\eta) - \mathbb{E}\widetilde{F}(\kappa)) = f(0, h, m, \beta) - \frac{\beta^2}{2}\int_0^1 qm(q)\,\mathrm{d}r(q)$$

where $h = \beta^{-1}\cosh^{-1}(\mathbb{E}_\sigma\sigma_1)$. This solution was originally obtained using the replica method. The preceding construction gives, at the least, a clear mathematical meaning to the objects involved. In particular, the notion of "ultra-metric zero-dimensional matrices," appears now to be equivalent to ultra-metric structures on the unit interval.

In a recent paper, Talagrand (2003) has proven that converse inequality is also true in the preceding equation, confirming that Parisi's solution yields the correct free energy in a large class of models of the SK type.

Ghirlanda–Guerra Relations

The appearance of a universal probabilistic structure in the asymptotics of these models may appear surprising. A partial explanation can be found in a set of remarkable identities between multi-overlap distributions that has been discovered first by Ghirlanda and Guerra (1998) in the context of SK models. If $\mu_{\beta,N}^{\otimes n}$ denotes the n-fold product Gibbs measure, the Ghirlanda–Guerra relations assert a recursion relation of the form

$$\begin{aligned}\mathbb{E}\mu_{\beta,N}^{\otimes n+1}&\left(D_N(\sigma^{n+1},\sigma^k)\le t|\mathcal{B}_n\right)\\ &= \frac{1}{n}\sum_{\ell\neq k}\mathbb{E}\mu_{\beta,N}^{\otimes n}\left(D_N(\sigma^\ell,\sigma^k)\le t|\mathcal{B}_n\right)\\ &\quad+\frac{1}{n}\mathbb{E}\mu_{\beta,N}^{\otimes 2}(D_N(\sigma^1,\sigma^2)\le t|\mathcal{B}_n)+o(1)\end{aligned}$$

These relations hold generically for Gaussian mean-field models, with D_N being the distance through which the covariance is defined. The proof of these relations is based on Gaussian integration-by-parts formulas, and concentration of measure inequalities. In the case of the GREM models, where D_N is ultra-metric, these recursions are sufficient to determine all n-replica overlap distributions in terms of the 2-replica distribution. On the other hand, the set of n-replica overlap distributions determines the law of the process $\mathcal{K}$ and thus the geometry of the Gibbs measure. In particular, they leave time changes of Neveu's process as the only candidates for limit processes. In the case of the SK models, the same does not hold *a priori*, since the Hamming distance is not an ultra-metric. However, since the Parisi solution is correct, this suggests very strongly that asymptotically the overlap distances are almost surely (with respect to the Gibbs measure) ultra-metric. Then, the Ghirlanda–Guerra identities also imply that the geometry of the Gibbs measures is described by the same structure.

From Mean-Field to Lattice Models

One of the widely discussed issues in the theory of spin glasses is to what extent the results of mean-field theory are relevant for lattice models. This issue has been addressed elsewhere in this encyclopedia by Newman and Stein. Here, we will only mention a recent result of Franz and Toninelli (2004) that shows that the free energy of the SK model can be represented as the limit of the free energy of lattice models when the range of the interaction tends to zero while their strength tends to zero in an appropriate way (the so-called Kac models). This still leaves open many finer questions, but hints to the fact that mean-field theory bears at least some relevance for realistic spin glasses.

See also: Short-Range Spin Glasses: The Metastate Approach; Spin Glasses.

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Measure on Loop Spaces

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Introduction

Loop spaces have been considered for their geometric interest (Freed Daniel 1988) where the space of based loops on a compact Lie group is endowed with a Kählerian structure; see also the survey by L Gross (1988). The harmonic analysis on loop groups, developed by Pressley and Segal, is reviewed by Hsu (1997). Loop groups have also an impact in string theory (Bowick and Rajeev 1987). They are related to Yang–Mills theory (Levy 2003). A presentation of the history of measure on infinite-dimensional spaces has been given by P Malliavin (see Malliavin (1992) and references therein). The main problem is the construction of measures on the loop space which have quasi-invariance property. This has implications in representation theory (Neretin 1994, Jones 1995). Here we mainly concentrate on the nonlinear stochastic point of view and its interference with geometry. The geometrical study of the space of closed curves over a compact Riemannian manifold M, that is, the loop space over M, was initiated by Marston Morse in 1932. The loop space is itself a manifold where one can define a Laplace–Beltrami operator. A diffusion process can be considered on this manifold. Wiener defined the Brownian loop by the Fourier series

$$u(\tau) = \sum_{k \geq 1} \frac{\sin k\pi\tau}{k} G_k \qquad [1]$$

where the G_k are independent normal variables. The time evolution of the Wiener loop and the extension of the theory to the case of a compact Riemannian manifold of finite dimension has been considered by Airault and Malliavin (1996, and references therein). The Brownian loop evolutes in the time parameter t as a Brownian sheet where the independent random variables G_k are function of t.

Starting from the zero loop, one obtains at time t, a random loop, and the law of this loop gives a measure on the loop space. A construction of this measure with functional analysis on infinite-dimensional manifold was done by Gaveau and Mazet (1979). The tools of stochastic analysis are important to the subject. The loop space of continuous maps from the circle to the multiplicative group of complex numbers has a group structure, hence the term "loop group." On the loop group, we consider the multiplicative Brownian motion starting at one point of the circle and conditioned to come back at this point at time s. It defines a probability measure on the loop group. One can also consider the set of continuous maps from the circle to the set of complex numbers of modulus equal to 1. The loop group is the space of continuous closed paths on a Lie group. More generally, on a Riemannian manifold M, the Brownian motion on M defines a Wiener measure on the loops over M. To go from the path space to the loop space, an important tool is the quasisure analysis in infinite dimension. The quasisure analysis was developed by Airault and Malliavin (1996, and references therein) to obtain disintegrations of the Wiener measure and they have used this tool in 1992 to construct measures on the loop group. The main problems are:

1. The construction of heat kernel measures and the existence of a Brownian motion on the loop space, the existence of pinned Wiener measures obtained as the law of Brownian motions conditioned on the loops.
2. The quasi-invariance of these transition probability measures under translation, or multiplication if we have a multiplicative structure, or under the infinitesimal action of suitable vector fields. For the path space over the n-dimensional Euclidean space R^n, the Cameron–Martin theorem (1944) ensures the existence of a density which shows the quasi-invariance of the Wiener measure under translations. For the quasi-invariance, an important fact is the choice of the metric on the Cameron–Martin space. In the case of the Wiener measure, one considers the paths of finite energy, $\int_0^1 |h'(s)|^2 ds < +\infty$. This corresponds to the metric "1." P Malliavin (1989, and references therein) discussed the case of metrics α with $1/2 < \alpha < 1$.
3. To define the "good" Cameron subspace, that is, find the vector fields that yield integration-by-parts formulas. The question occurs whether the Cameron–Martin space depends on time. For the loop space, it has been proved by Driver (2003) that it is not the case. A time evolution of the tangent Cameron–Martin space could appear eventually.
4. The determination of the support of the measures (e.g., the Wiener measure) is carried by the set of Hölder functions of order $1/2 - \epsilon$.
5. The absolute continuity of the measures with respect to each other.

The Construction of Heat Measures on the Loop Space and Their Quasi-Invariance

The construction of measures giving a solution to the infinite-dimensional heat equation as well as the study of the quasi-invariance of the Wiener measure on the path space was started extensively in the work by Bismut, followed by Gross (1998), then by Aida and Elworthy (1995) where the loop group is a suitable manifold to extend to infinite-dimensional manifolds the log-Sobolev inequalities, by Malliavin and Malliavin (1992, and references therein) where the measures on the path space and the path group have been studied. Consider a compact Lie group G with unit e and let $\mathcal{G}$ be its Lie algebra. From the $\mathcal{G}$-valued Brownian motion, one can construct a family of measures $(\mu_t^e)_{t\geq 0}$ on the path space. These measures μ_t^e are the images of the Wiener measure on $\mathcal{G}$ through the Ito map

$$dg_x(\tau) = \sqrt{t}\, g_x(\tau)dx(\tau) \quad \text{with } g_x(0) = e \qquad [2]$$

The convolution of two measures μ_t^e and $\mu_{t'}^e$ is equal to $\mu_{t+t'}^e$. By choosing the initial value of the path randomly distributed according to the Haar measure on G, it defines a family of measures $(\mu_t)_{t\geq 0}$ on the path space with

$$\int f(\gamma)\, \mu_t(d\gamma) = \int dg \int f(g\gamma)\mu_t^e(d\gamma)$$

The Laplacian on the path group is defined by

$$(\Delta_P f)(g) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\int f(g\gamma)\mu_\epsilon(d\gamma) - f(g)\right]$$

The heat equation is valid for the measures $(\mu_t)_{t\geq 0}$ on the paths,

$$\frac{\partial}{\partial t}\int f(g)\mu_t(dg) = \int (\Delta_P f)(g)\mu_t(dg)$$

Moreover, there is a quasi-invariance density $k_{g_0}(g)$ defined on the path group (g_0 and g are paths with values in G) such that

$$\mu_t(g_0 A) = \int_A k_{g_0}(g)\mu_t(dg)$$

where $g_0 A$ is the translated on the left of the subset A in the path space over G. This is a generalization to the path space of the classical Cameron–Martin theorem. Then, one can consider the loop space. The free loop space is the set of continuous maps g from $[0,1]$ to G such that $g(0)=g(1)$, and the loop space with a base point is the set of maps such that $g(0)=g(1)=m$ is fixed. One can define the pinned Brownian motion on the group G to obtain the pinned Wiener measures $(\mu_t^{L_e})_{t\geq 0}$ on the loop group (Malliavin and Malliavin 1992, Driver and Srimurthy 2001). Denote by $p_t(g)$ the solution of the heat equation on the group G. Let g be a map from $[0,1]$ to the finite-dimensional Lie group G. For $\tau_1,\tau_2,\ldots,\tau_n\in[0,1]$, consider the evaluations of the map g, $g_{\tau_1}, g_{\tau_2},\ldots,g_{\tau_n}\in G$, Let f be a real function defined on G and denote by dg the Haar measure on G. The measure $\mu_t^{L_e}$ on the loop group is given by

$$\begin{aligned}\int f(g_{\tau_1}, g_{\tau_2},\ldots,g_{\tau_n})\, d\mu_t^{L_e}(g) &= \int f(g_1,g_2,\ldots,g_n)p_{t\tau_1}(g_1)p_{t(\tau_2-\tau_1)}(g_1^{-1}g_2)\cdots \\ &\quad\times p_{t(\tau_n-\tau_{n-1})}(g_{n-1}^{-1}g_n)p_{t(1-\tau_n)}(g_n)\, dg_1\cdots dg_n\end{aligned}$$

From $\mu_t^{L_e}$, one defines a measure μ_t^L on the free loops by taking the mean over G as

$$\int f(\gamma)\mu_t^L(d\gamma) = \int_G dg \int f(g\gamma)\mu_t^{L_e}(d\gamma)$$

The quasi-invariance property for the pinned Wiener measure was proved by Malliavin and Malliavin (1992).

When the measures $(\mu_t^L)_{t\geq 0}$ are obtained by conditioning and quasisure analysis, we have heat kernel measures. The case of heat kernel measures defined on the loop group has been studied by Airault and Malliavin by disintegrating the measures on the path space and using the quasisure analysis. The Laplacian on the loop group is defined as it has been for the Laplacian on the path space,

$$(\Delta_L f)(g) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\int f(gg_1)\mu_\epsilon^L(dg_1) - f(g)\right]$$

but now the heat equation has a Kac's potential Φ_t defined on the loops. On the loop group, the heat equation is

$$\frac{\partial}{\partial t}\int f(l)\mu_t^L(dl) = \int [(\Delta_L f)(l) + \Phi_t(l)f(l)]\mu_t^L(dl) \qquad [3]$$

where

$$\begin{aligned}\Phi_t(l) &= \frac{1}{t^2}\left\|\int_0^1 dl(s)l(s)^{-1}\right\|_{\mathcal{G}}^2 - 2\frac{d}{dt}\log p_t(e) \\ &\quad - \frac{1}{t}\dim\mathcal{G}\end{aligned}$$

The case of the circle, $G=R/2\pi Z$, is interesting. The law of the functional

$$\int_0^1 dl(s)l(s)^{-1}$$

is given in Airault and Malliavin (1996, and references therein). Moreover, the study of the heat

measures over the loop group of $R/2\pi Z$ brings new identities on the classical Jacobi theta function

$$p_t(\theta) = 1 + 2\sum_{n\geq 1} \cos(n\theta)\,e^{-n^2 t/2} \quad \text{at } \theta = 0$$

Let

$$c_t = -2\frac{d}{dt}\log p_t(0) - \frac{1}{t}$$

The following system of differential equations is given by Airault–Malliavin (1996, and references therein):

$$c_t = -\frac{1}{t^2}\sum_{n\in Z} a_n(t)$$

$$\frac{d}{dt}a_n(t) = \frac{1}{2}c_t a_n(t) + \frac{2\pi^2 n^2}{t^2}a_n(t)$$

To pass from path space to loop space, it is convenient to use the "tubular chart" introduced by Gross and the quasisure analysis developed by Airault–Malliavin. Let $\Phi : \gamma \to \gamma(1)\gamma(0)^{-1}$ from the path space to the group G; then the free loop space over G is $\Phi^{-1}(e)$. There exists a neighborhood V of the neutral of G such that $\Phi^{-1}(V)$ is diffeomorphic to $V \times L(G)$, the product of V with the loop space over G. With this diffeomorphism, one can disintegrate the measures on the path space and obtain the measures on the loop space. The Cameron–Martin formula on the path space of the group G is obtained from the Cameron–Martin formula for the Wiener space and the Ito's map. Let γ be a differentiable path with finite energy on G, that is,

$$\int_0^1 \left\| \gamma(s)^{-1}\frac{d}{ds}\gamma(s)\right\|_{\mathcal{G}}^2 < +\infty$$

it holds

$$\int f(\gamma g)\mu_t(dg) = \int f(g)k_\gamma(g)\mu_t(dg)$$

Let us denote by $(|)_{\mathcal{G}}$ the Euclidean scalar product on the Lie algebra $\mathcal{G}$; then the density is given by

$$k_\gamma(g) = \exp\left[\frac{1}{t}\int_0^1 \left(\gamma(s)^{-1}\frac{d}{ds}\gamma(s)|dg(s)g(s)^{-1}\right)_{\mathcal{G}} - \frac{1}{2t}\int_0^1 \left\|\gamma(s)^{-1}\frac{d}{ds}\gamma(s)\right\|_{\mathcal{G}}^2 ds\right]$$

The previous approach relies on the heat equation on the loop space. Thus, the metric on the Cameron–Martin loop or path space is important. The problem of quasi-invariance for metrics α with $1/2 < \alpha < 1$ relates to the random series

$$u_\alpha(\tau) = \sum_{k\geq 1}\frac{\sin k\pi\tau}{k^\alpha}G_k \qquad [4]$$

where the G_k are independent normal variables. Driver (2003) solved the problem for $1/2 < \alpha < 1$ by Riemannian geometry in infinite dimension. The Ricci curvature appears in the integration-by-parts formulas on the loop space. The case of the metric 1/2 is out of reach. Fang (1999) calculated the Ricci curvature of the loop manifold for metrics $\alpha > 1/2$ and showed that when $\alpha \to 1/2$, these Ricci curvatures tend to a limit. Another presentation of the problem is that of Pickrell (1987), where he obtains a family of quasi-invariant measures on Grassmannians.

Given a family of measures $(\mu_t)_{t\geq 0}$ on the path space of a Riemannian manifold, one defines a heat operator as a family $(\mathcal{L}_t)_{t\geq 0}$ of operators depending upon $t \in [0, +\infty[$ such that

$$\int \mathcal{L}_t F\, d\mu_t = \frac{d}{dt}\int F\, d\mu_t \qquad [5]$$

where F is a function defined on the path space. The heat equation with a potential as [3] gives an example of a heat operator. Heat operators have been constructed for the path space over R^n by Airault–Malliavin, obtaining, after an integration by parts on the path space, a heat operator of first order. This introduces the notion of dilatation vector fields on the path space. In the case of the flat Wiener space, to each point x in the path space is associated the dilatation vector field Y such that $(Yf)(x) = (x|(\text{grad} f)(x))$. This gives a rescaling of the Wiener measure under dilatations. This idea has been exploited by Mancino (1999), who extended the method to free loop groups.

Integration-by-Parts Formulas

The Cameron–Martin space plays the role of the tangent space to the Wiener space. The integration-by-parts formulas are an infinitesimal version of the Cameron–Martin quasi-invariance property. Let G be a compact Lie group or any product of R^n by a compact Lie group. For a vector field z, the differentiation on the right $\partial_z^{\text{right}}$ and differentiation on the left ∂_z^{left} are given by

$$\partial_z^{\text{left}}F(p) = \lim_{\epsilon\to 0}\frac{F(\exp(\epsilon z)p) - F(p)}{\epsilon}$$

and

$$\partial_z^{\text{right}} F(p) = \lim_{\epsilon \to 0} \frac{F(p \exp(\epsilon z)) - F(p)}{\epsilon}$$

The operator $\partial_z^{\text{right}}$ commutes with the translation on the left, for a translation τ_h^{left}, then $\partial_z^{\text{right}}(F o \tau_h^{\text{left}}) = (\partial_z^{\text{right}} F) o \tau_h^{\text{left}}$ and vice versa for ∂_z^{left}.

For the measures on the path space or loop space, the problem is to prove the integration-by-parts formulas. On the path spaces on G, let μ_{P_e} be the Wiener measure on the set of paths starting from e, there exists a density k_z such that $E[\exp(ck_z)]$ is finite and

$$\int_{P_e(G)} \partial_z^{\text{left}} F(g) \, d\mu_{P_e}(g) = \int_{P_e(G)} F(g) k_z \, d\mu_{P_e}(g)$$

The density k_z is defined on the path space by

$$k_z(g) = \int_0^1 < g(t) z'(t) g(t)^{-1}, d\omega(t) >$$

This was proved by a number of authors (see, e.g., Pickrell (1987) and, in a geometrical context, Cruzeiro and Malliavin (1996)).

The existence of a density for the differentiation on the left is valid for any Lie group. This is not true for the differentiation on the right. If G is noncompact or is not the product of R^n by a compact Lie group, the existence of k_z is not proved on the right. This comes from the fact that the map Ad defined on the path group as a parallel transport does not preserve the Cameron–Martin subspace. In the case where G is not a product of a flat space by a compact Lie group, the Cameron space, which is a kind of "tangent space" to the infinite-dimensional loop manifold, is not closed under the Lie bracket of vector fields.

The integration-by-parts formulas are obtained with the stochastic calculus of variation. On a group G, consider $Y_1, Y_2, \ldots, Y_p$, p independent left-invariant vector fields. Let $\mathcal{G}$ be the Lie algebra of G. The second-order differential operator $\triangle = \sum_{j=1}^{p} Y_j^2$ defines a left-invariant diffusion $g_\omega(t)$ on the group G with the stochastic equation $dg_\omega(t) = g_\omega(t)\left[\sum_k (Y_k)_e o \, d\omega^k\right]$ where (ω_k) are independent Brownian motions on the Euclidean space $\mathcal{G}$. In the work by Malliavin and Malliavin (1992, and references therein), the stochastic calculus of variation is done with the right-invariant connection on the Lie group by setting

$$\phi^{\text{right}} = \frac{d}{d\epsilon_{|\epsilon=0}} (g_{\omega+\epsilon h}) o g_\omega^{-1}$$

where h is a differentiable function of t with values in the Lie algebra $\mathcal{G}$, with finite energy $\int_0^1 |h'(s)|^2 \, ds < +\infty$. By taking the derivative with respect to ϵ in the Stratonovitch equation

$$g^\epsilon(t)^{-1} o \, dg^\epsilon(t) = d\omega(t) + \epsilon h'(t) \, dt$$

and letting $\epsilon = 0$, it turns out that ϕ^{right} is a differentiable function of t and its derivative is given by

$$\frac{d}{dt} \phi^{\text{right}}(t) = g_\omega(t) h'(t) g_\omega(t)^{-1}$$

The situation is not the same for

$$\phi^{\text{left}} = \frac{d}{d\epsilon_{|\epsilon=0}} g_\omega^{-1} o (g_{\omega+\epsilon h})$$

where $d\phi^{\text{left}}(t)$ is a stochastic differential. This generalizes to an arbitrary Riemannian manifold using a coupling of connections (see Airault and Malliavin (1996), and references therein). The construction of the appropriate Cameron subspace, that is, the choice of the infinitesimal action of vector fields on the measure, is of importance. In the commutative case of the path space over R^n, the classical Cameron–Martin subspace of paths h such that $\int_0^1 |h'(s)|^2 \, ds < +\infty$ is time invariant. To define the vector fields acting on the path (or loop) space over M, it is necessary to consider the geometry of the manifold M. The infinitesimal transformations which preserve the Riemannian metric are called Riemannian connections. In the case where M is a group, the natural connections are those defined by the parallelism on the group. For a Riemannian manifold, Driver proved the existence of integration-by-parts formulas for the measures on the path space of M when M is endowed with a torsion skew-symmetric connection. The Levi-Civita connection, since it is torsionless, is of course a Driver (2003) connection. If the connection is not skew-symmetric, then two coupled connections permit study of the ϵ-variation or "reduced variation" of a path, and one obtains a Cameron–Martin formula on the path and on the loop space of the Riemannian manifold M (Fang 1999). The method of reduced variation can be used to obtain the integration-by-parts formulas over path and loop spaces. Another approach to the quasi-invariance problem, using two-parameter processes, has been provided by Norris (1995).

The Support of the Measures and Absolute Continuity with Respect to Each Other

Given a Riemannian manifold M, let $(\mu_t)_t$ be the heat kernel measures on the path space of M and let $(\rho_t)_t$ be heat kernel measures on the loop space of M; the question arises whether ρ_t is absolutely continuous

with respect to μ_t. For a connected compact Lie group G, consider the path and loop groups on G. The pinned Wiener measure on the loop group is defined as the law of a G-valued Brownian motion starting at e and conditioned to end at e, and the heat kernel measure is the endpoint distribution of Brownian motion on the loop group.

It has been shown (Driver and Srimurthy 2001) that the heat kernel measure is absolutely continuous with respect to the pinned Wiener measure, and that the Radon–Nikodym derivative is bounded. This proof relies on the heat formula with a potential [3], which is satisfied by the heat kernel measure. They give a new proof of this heat formula. When the group G is simply connected, Aida and Driver (2000) prove that the heat kernel measure over a based loop group, constructed by using the Brownian motion is equivalent to the Brownian bridge measure over a based loop group. When G is the circle, the Radon–Nikodym derivative of the heat kernel measure with respect to the pinned Wiener measure can be calculated in terms of the Jacobi theta function (Driver and Srimurthy 2001). On the loop space of R^n, at time t, the two measures, "heat kernel" and "pinned Wiener" are the same.

See also: Abelian and Nonabelian Gauge Theories Using Differential Forms; Lie Groups: General Theory; Malliavin Calculus; Path Integrals in Noncommutative Geometry.

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Metastable States

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Introduction

The theory of metastability studies the states of the matter which "should not be there," but which still can be observed, albeit for only a short time. One example is water, cooled below the zero temperature. This supercool water can stay liquid, but not for a long time, and it then freezes abruptly. Such states are called metastable. They are not equilibrium states; at negative temperatures the only equilibrium state of water is ice. Physically, these metastable states are produced from the equilibrium states by slowly changing the external parameters, such as the temperature (or magnetic field): one takes, for example, water (extremely purified) at low positive temperature, $T > 0$, and then lowers the

temperature slowly to negative values $T < 0$. Thus, the family of metastable states, $\mathfrak{s}_T, T < 0$, should be thought as a continuation of the family $\mathfrak{s}_T, T > 0$ of equilibrium states through the point of phase transition $T_c = 0$, at which critical temperature these states cease to exist as equilibrium states.

Below we will present rigorous results, which validate the above picture for the case of the 2D Ising model. They are contained in Schonmann and Shlosman (1998). The relevant external parameter in this case will be the magnetic field, h.

It turns out that the lifetime of metastable states is determined by the quantities given by the Wulff construction.

Equilibrium States and Dynamics

Let us denote the set $\{-1, +1\}^{\mathbb{Z}^2}$ of the Ising model configurations σ by Ω. Two configurations are specially relevant, the one with all spins -1 and the one with all spins $+1$. We will use the simple notation $-$ and $+$ to denote them.

Observables are just functions on Ω. Local observables are those which depend only on the values of finitely many spins.

We will consider the formal Hamiltonian

$$H_h(\sigma) = -\sum_{x,y \text{ n.n.}} \sigma(x)\sigma(y) - h\sum_x \sigma(x) \qquad [1]$$

where $h \in \mathbb{R}^1$ is the external field and $\sigma \in \Omega$ is a generic configuration. We define, for each set $\Lambda \subset\subset \mathbb{Z}^2$ and each boundary condition $\xi \in \Omega$,

$$H_{\Lambda,\xi,h}(\sigma) = -\sum_{\substack{x,y \text{ n.n.}\\ x,y\in\Lambda}} \sigma(x)\sigma(y) - \sum_{\substack{x,y \text{ n.n.}\\ x\in\Lambda, y\notin\Lambda}} \sigma(x)\xi(y) - h\sum_{x\in\Lambda} \sigma(x)$$

The "grand canonical Gibbs measure" in Λ with boundary condition ξ under external field h and at temperature T is defined on Ω_Λ as

$$\mu_{\Lambda,\xi,T,h}(\sigma) = Z^{-1}_{\Lambda,\xi,T,h} \exp(-\beta H_{\Lambda,\xi,h}(\sigma))$$

where $\beta = T^{-1}$, and the partition function $Z_{\Lambda,\xi,T,h}$ is a normalization, chosen such that $\mu_{\Lambda,\xi,T,h}(\Omega_\Lambda) = 1$. The equilibrium states are obtained by taking the thermodynamic limit $\lim_{\Lambda\to\mathbb{Z}^2} \mu_{\Lambda,\xi,T,h}$. We will be interested in the states

$$\mu_{\pm,T,h} = \lim_{\Lambda\to\mathbb{Z}^2} \mu_{\Lambda,\pm,T,h}$$

corresponding to $(\pm)$-boundary conditions. If $h \neq 0$, then $\mu_{-,T,h} = \mu_{+,T,h}$, so it will be denoted simply by $\mu_{T,h}$. If $h = 0$, the same is true if the temperature is larger than or equal to a critical value $T_c = T_c$, and is false for $T < T_c$, in which case one says that there is phase coexistence. The measure $\mu_{+,T,0} \equiv \mu_{+,T}$ is called the $(+)$-phase, and $\mu_{-,T}-$ the $(-)$-phase.

For an observable f we will denote by $\langle f\rangle_*$ its expected value in the state μ_*, that is, the integral $\int f \mathrm{d}\mu_*$. In particular, the spontaneous magnetization $m^*(T)$ equals by definition to $\langle\sigma(0)\rangle_{+,T}$.

Next, we need to supply the Ising model with the time evolution. For this we will use the Glauber dynamics. It is a Markov process on Ω, whose generator, L, acts on a generic local observable f as

$$(Lf)(\sigma) = \sum_{x\in\mathbb{Z}^2} c(x,\sigma)(f(\sigma^x) - f(\sigma))$$

where σ^x is the configuration obtained from σ by flipping the spin at the site x to the opposite value, and $c(x,\sigma)$ is the rate of the flip of the spin at the site x when the system is in the state σ. In words, one can say that the dynamics proceeds as follows: at every site x the spin $\sigma(x)$ is flipped randomly, independently of all others, with the rate $c(x,\sigma)$, where σ is the current configuration. Common examples are "metropolis dynamics":

$$c_h(x,\sigma) = \exp(-\beta(\Delta_x H_h(\sigma))^+)$$

or "heat bath dynamics":

$$c_h(x,\sigma) = [1 + \exp(\beta\Delta_x H_h(\sigma))]^{-1}$$

Here $(a)^+ = \max\{a, 0\}$, and $\Delta_x H_h(\sigma) = H_h(\sigma^x) - H_h(\sigma)$. The spin flip system thus obtained will be denoted by $(\sigma^\xi_{T,h;t})_{t\geq 0}$, where ξ is the initial configuration at time $t = 0$. If this initial configuration is selected at random according to a probability measure ν, then the resulting process is denoted by $(\sigma^\nu_{T,h;t})_{t\geq 0}$. It is known that the Gibbs measures are invariant with respect to the stochastic Ising models. Moreover,

$$\sigma^-_{T,h;t} \to \mu_{-,T,h}, \sigma^+_{T,h;t} \to \mu_{+,T,h}, \quad \text{as } t\to\infty$$

We will be interested in the case when h is positive, though small. Then there is only one invariant state, $\mu_{+,T,h}$, so the state $\mu_{-,T,h}$ is equal to $\mu_{+,T,h}$, and $\sigma^-_{T,h;t} \to \mu_{+,T,h}$, as $t\to\infty$. (One should intuitively think about the state $\sigma^-_{T,h;t}$ for t small as the supercooled but liquid water, thinking about the state $\mu_{+,T,h}$ to be ice.) We want to control the convergence of the temporal state $\sigma^-_{T,h;t}$ to the equilibrium, $\mu_{+,T,h}$, and to see, if possible, that during some (long) initial time the state $\sigma^-_{T,h;t}$ looks very similar to the $(-)$-phase $\mu_{-,T}$, while after some time threshold it changes suddenly and looks quite similar to the state $\mu_{+,T,h}$. It turns out that all the above features can indeed be established rigorously.

If one starts to simulate the above dynamics on a computer, then the picture observed would be the following: one would see that droplets of the (+)-phase are created in the midst of (−)-phase droplets, which are there for a while, and then disappear. That process goes on for a while, until a big enough (+)-droplet is born; this one then starts to grow and eventually fills up all the display.

The Life Span of Metastable States

Let us define the "critical time exponent" $\lambda_c = \lambda_c(T)$ by

$$\lambda_c = \frac{w_T}{12m^*(T)T} \qquad [2]$$

where $w_T = w_{\mathfrak{W}_T}$ is the value of the surface energy of the Wulff curve of our 2D Ising model at the temperature T:

$$w_T = \mathcal{W}_T(\mathfrak{W}_T)$$

Suppose now that $T < T_c, h > 0$. Let ν be either the (−)-phase $\mu_{-,T}$ or $\delta_{\{\sigma=-\}}$. (In fact, any ν "between" these two states would go.) Then the following happens.

1. If $0 < \lambda < \lambda_c$, then for each $n \in \{1, 2, \ldots\}$ and for each local observable f,

$$\mathbb{E}\left(f\left(\sigma^{\nu}_{T,h;t=\exp\{\lambda/h\}}\right)\right) = \sum_{j=0}^{n-1} b_j(f)h^j + O(h^n) \qquad [3]$$

where

$$b_j(f) = \lim_{h\to 0-} \frac{\mathrm{d}^j \langle f\rangle_{-,T,h}}{\mathrm{d}h^j}$$

(We stress that in the last relation we are using the Gibbs states corresponding to the negative values of the magnetic field.) In particular,

$$\mathbb{E}\left(\sigma^{\nu}_{T,h;t=\exp\{\lambda/h\}}(0)\right) = -m^*(T) + O(h) \qquad [4]$$

2. If $\lambda > \lambda_c$, then for any finite positive C there is a finite positive C_1 such that for every local observable f,

$$\left|\mathbb{E}\left(f\left(\sigma^{\nu}_{T,h;t=\exp\{\lambda/h\}}\right)\right) - \langle f\rangle_{T,h}\right| \leq C_1\|f\|\exp\left\{-\frac{C}{h}\right\} \qquad [5]$$

The relation [3] implies that the family of nonequilibrium states $\langle\cdot\rangle^{\nu}_{T,h;\lambda}, h > 0$, defined for every local observable f by

$$\langle f\rangle^{\nu}_{T,h;\lambda} = \mathbb{E}\left(f\left(\sigma^{\nu}_{T,h;t=\exp\{\lambda/h\}}\right)\right)$$

is a C^{∞}-continuation of the curve $\{\langle\cdot\rangle_{-,T,h}, h \leq 0\}$ of equilibrium states. This is true for every $0 < \lambda < \lambda_c$ and every ν as above. The states $\langle\cdot\rangle^{\nu}_{T,h;\lambda}$ are the "metastable states" we are looking for. The relations [3] and [4] should be interpreted in the sense that before the time $\exp\{\lambda_c/h\}$ our temporal state is still "liquid," while [5] means that after the time $\exp\{\lambda_c/h\}$ freezing happens. So one can think about the quantity $\exp\{\lambda_c/h\}$ as being the life span of the metastable state.

This theorem was obtained in Schonmann and Shlosman (1998). Let us explain the heuristics behind it. It has two ingredients. The first one is that the transition to the equilibrium is going via creation of droplets of the (+)-phase. The second one is that once such a droplet is created by a thermal fluctuation, with the size exceeding a certain critical value, it does not die out, but grows further, with a speed v of the order of h. (This second belief can be expected to be correct only in dimension 2.) Let us see how these two hypotheses can give us the right answer. To get to the equilibrium we have to overcome the energy barrier, by creating a large droplet of the (+)-phase. Subcritical droplets are constantly created by thermal fluctuations in the metastable phase, but they tend to shrink. On the other hand, once a supercritical droplet is created due to a larger fluctuation, it will grow and drive the system to the stable phase. Indeed, the energy $\Phi(\mathfrak{m})$ of an $\mathfrak{m}$-shaped droplet of the (+)-phase in the sea of (−)-phase equals $\mathcal{W}_T(\mathfrak{m}) - 2m^*(T)h\,\mathrm{vol}(\mathfrak{m})$. For small $\mathfrak{m}$ the functional $\Phi(\mathfrak{m})$ decreases as $\mathfrak{m}$ shrinks, while for large $\mathfrak{m}$ the functional $\Phi(\mathfrak{m})$ decreases as $\mathfrak{m}$ grows. Its saddle point $\mathfrak{m}_{\mathrm{sdl}}$ is precisely the Wulff shape. Since the minimal height of the barrier is $\Phi(\mathfrak{m}_{\mathrm{sdl}})$, one predicts the rate of creation of a critical droplet with center at a given place to be

$$\exp\left\{-\frac{\Phi(\mathfrak{m}_{\mathrm{sdl}})}{T}\right\} = \exp\left\{-\frac{w_T}{4m^*(T)T}\right\}$$

Comparing with [2], we see that we miss the correct answer

$$\exp\left\{-\frac{w_T}{12m^*(T)T}\right\}$$

by a factor of 1/3. The reason for that is the following. Note that we are concerned with an infinite system, and we are observing it through a

local function f, which depends on the spins in a finite set supp (f). For us, the system will have relaxed to equilibrium once supp (f) is covered by a big droplet of the (+)-phase, which appeared spontaneously somewhere and then grew, as discussed above. We want to estimate how long we have to wait for the probability of such an event to be close to 1. If we suppose that the radius of the supercritical droplet grows with a speed v, then we can see that the region in spacetime, where a droplet which covers supp (f) at time t could have appeared, is, roughly speaking, a cone with vertex in supp (f) and which has as base the set of points which have time coordinate 0 and are at most at distance tv from supp (f). The volume of such a cone is of the order of $(vt)^2t$. The order of magnitude of the relaxation time, t_{rel}, at which the region supp (f) starts to be covered by a large droplet can now be obtained by solving the equation

$$(vt_{\text{rel}})^2 t_{\text{rel}} \exp\left\{-\frac{\Phi(\mathfrak{m}_{\text{sdl}})}{T}\right\} \sim 1$$

This gives us what we want:

$$t_{\text{rel}} \sim v^{-2/3} \exp\left\{\frac{1}{3}\frac{\Phi(\mathfrak{m}_{\text{sdl}})}{T}\right\}$$

See also: Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; Large Deviations in Equilibrium Statistical Mechanics; Wulff Droplets.

Further Reading

Schonmann RH and Shlosman S (1998) Wulff droplets and the metastable relaxation of the kinetic Ising models. *Communications in Mathematical Physics* 194: 389–462.

Minimal Submanifolds

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Introduction

Soap films, soap bubbles, and surface tension were extensively studied by the Belgian physicist and inventor (the inventor of the stroboscope) Joseph Plateau in the first half of the nineteenth century. At least since his studies, it has been known that the right mathematical model for soap films are minimal surfaces – the soap film is in a state of minimum energy when it is covering the least possible amount of area. Minimal surfaces and equations like the minimal surface equation have served as mathematical models for many physical problems.

The field of minimal surfaces dates back to the publication in 1762 of Lagrange's famous memoir "Essai d'une nouvelle méthode pour déterminer les maxima et les minima des formules intégrales indéfinies." Euler had already, in a paper published in 1744, discussed minimizing properties of the surface now known as the catenoid, but he only considered variations within a certain class of surfaces. In the almost one-quarter of a millennium that has past since Lagrange's memoir, the subject of minimal surfaces has remained a vibrant area of research and there are many reasons why. The study of minimal surfaces was the birthplace of regularity theory. It lies on the intersection of nonlinear elliptic PDE, geometry, topology, and general relativity.

In what follows we give a quick tour through many of the classical results in the field of minimal submanifolds, starting at the definition.

The field of minimal surfaces remains extremely active and has very recently seen major developments that have solved many longstanding open problems and conjectures; for more on this, see the expanded version of this survey (Colding and Minicozzi II, 2005). See also the recent surveys (Meeks III and Perez 2004, Perez 2005), and the expository article (Colding and Minicozzi II 2003).

Throughout this survey, we refer to Colding and Minicozzi II (1999) for references unless otherwise noted.

Part 1. Classical and Almost Classical Results

Let $\Sigma \subset \boldsymbol{R}^n$ be a smooth k-dimensional submanifold (possibly with boundary) and $C_0^\infty(N\Sigma)$ the space of all infinitely differentiable, compactly supported, normal vector fields on Σ. Given Φ in $C_0^\infty(N\Sigma)$, consider the one-parameter variation

$$\Sigma_{t,\Phi} = \{x + t\,\Phi(x) | x \in \Sigma\} \qquad [1]$$

The so-called first variation formula of volume is the equation (integration is with respect to d(vol)

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathrm{Vol}(\Sigma_{t,\Phi}) = \int_\Sigma \langle \Phi, \boldsymbol{H} \rangle \qquad [2]$$

where $\boldsymbol{H}$ is the mean curvature (vector) of Σ. (When Σ is noncompact, then $\Sigma_{t,\Phi}$ in [2] is replaced by

$\Gamma_{t,\Phi}$, where Γ is any compact set containing the support of Φ.) The submanifold Σ is said to be a "minimal" submanifold (or just minimal) if

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathrm{Vol}(\Sigma_{t,\Phi}) = 0 \quad \text{for all } \Phi \in C_0^\infty(N\Sigma) \qquad [3]$$

or, equivalently by [2], if the mean curvature $\boldsymbol{H}$ is identically zero. Thus, Σ is minimal if and only if it is a critical point for the volume functional. (Since a critical point is not necessarily a minimum, the term "minimal" is misleading, but it is time honored. The equation for a critical point is also sometimes called the Euler–Lagrange equation.)

Suppose now, for simplicity, that Σ is an oriented hypersurface with unit normal $\boldsymbol{n}_\Sigma$. We can then write a normal vector field $\Phi \in C_0^\infty(N\Sigma)$ as $\Phi = \phi \boldsymbol{n}_\Sigma$, where function ϕ is in the space $C_0^\infty(\Sigma)$ of infinitely differentiable, compactly supported functions on Σ. Using this, a computation shows that if Σ is minimal, then

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0} \mathrm{Vol}(\Sigma_{t,\phi \boldsymbol{n}_\Sigma}) = -\int_\Sigma \phi\, L_\Sigma \phi \qquad [4]$$

where

$$L_\Sigma \phi = \Delta_\Sigma \phi + |A|^2 \phi \qquad [5]$$

is the second variational (or Jacobi) operator. Here, Δ_Σ is the Laplacian on Σ and A is the second fundamental form. So $|A|^2 = \kappa_1^2 + \kappa_2^2 + \cdots + \kappa_{n-1}^2$, where $\kappa_1, \ldots, \kappa_{n-1}$ are the principal curvatures of Σ and $\boldsymbol{H} = (\kappa_1 + \cdots + \kappa_{n-1})\,\boldsymbol{n}_\Sigma$. A minimal submanifold Σ is said to be stable if

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0} \mathrm{Vol}(\Sigma_{t,\Phi}) \geq 0 \quad \text{for all } \Phi \in C_0^\infty(N\Sigma) \qquad [6]$$

Integrating by parts in [4], we see that stability is equivalent to the so-called stability inequality

$$\int |A|^2 \phi^2 \leq \int |\nabla \phi|^2 \qquad [7]$$

More generally, the "Morse index" of a minimal submanifold is defined to be the number of negative eigenvalues of the operator L. Thus, a stable submanifold has Morse index zero.

The Gauss Map

Let $\Sigma^2 \subset \boldsymbol{R}^3$ be a surface (not necessarily minimal). The Gauss map is a continuous choice of a unit normal $\boldsymbol{n}: \Sigma \to S^2 \subset \boldsymbol{R}^3$. Observe that there are two choices of such a map $\boldsymbol{n}$ and $-\boldsymbol{n}$ corresponding to a choice of orientation of Σ. If Σ is minimal, then the Gauss map is an (anti) conformal map since the eigenvalues of the Weingarten map are κ_1 and $\kappa_2 = -\kappa_1$. Moreover, for a minimal surface

$$|A|^2 = \kappa_1^2 + \kappa_2^2 = -2\,\kappa_1 \kappa_2 = -2\,K_\Sigma \qquad [8]$$

where K_Σ is the Gauss curvature. It follows that the area of the Gauss map is a multiple of the total curvature.

Minimal Graphs

Suppose that $u: \Omega \subset \boldsymbol{R}^2 \to \boldsymbol{R}$ is a C^2 function. The graph of u

$$\mathrm{Graph}_u = \{(x, y, u(x,y)) \mid (x,y) \in \Omega\} \qquad [9]$$

has area

$$\begin{aligned} \mathrm{Area}(\mathrm{Graph}_u) &= \int_\Omega |(1, 0, u_x) \times (0, 1, u_y)| \\ &= \int_\Omega \sqrt{1 + u_x^2 + u_y^2} \\ &= \int_\Omega \sqrt{1 + |\nabla u|^2} \end{aligned} \qquad [10]$$

and the (upward pointing) unit normal is

$$\boldsymbol{n} = \frac{(1, 0, u_x) \times (0, 1, u_y)}{|(1, 0, u_x) \times (0, 1, u_y)|} = \frac{(-u_x, -u_y, 1)}{\sqrt{1 + |\nabla u|^2}} \qquad [11]$$

Therefore, for the graphs $\mathrm{Graph}_{u+t\eta}$ where $\eta | \partial\Omega = 0$, we get that

$$\mathrm{Area}(\mathrm{Graph}_{u+t\eta}) = \int_\Omega \sqrt{1 + |\nabla u + t\,\nabla \eta|^2} \qquad [12]$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}t}_{t=0} \mathrm{Area}(\mathrm{Graph}_{u+t\eta})$$

$$= \int_\Omega \frac{\langle \nabla u, \nabla \eta \rangle}{\sqrt{1 + |\nabla u|^2}} = -\int_\Omega \eta\, \mathrm{div}\left(\frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) \qquad [13]$$

It follows that the graph of u is a critical point for the area functional if and only if u satisfies the divergence form equation

$$\mathrm{div}\left(\frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = 0 \qquad [14]$$

Next we want to show that the graph of a function on Ω satisfying the minimal surface equation, that is, satisfying [14], is not just a critical point for the area functional but is actually area minimizing amongst surfaces in the cylinder $\Omega \times \boldsymbol{R} \subset \boldsymbol{R}^3$. To show this, extend first the unit normal $\boldsymbol{n}$ of the graph in [11] to a vector field, still

denoted by $\boldsymbol{n}$, on the entire cylinder $\Omega \times \boldsymbol{R}$. Let ω be the 2-form on $\Omega \times \boldsymbol{R}$ given that for $X, Y \in \boldsymbol{R}^3$

$$\omega(X, Y) = \det(X, Y, \boldsymbol{n}) \qquad [15]$$

An easy calculation shows that

$$\mathrm{d}\omega = \frac{\partial}{\partial x}\left(\frac{-u_x}{\sqrt{1+|\nabla u|^2}}\right) + \frac{\partial}{\partial y}\left(\frac{-u_y}{\sqrt{1+|\nabla u|^2}}\right) = 0 \qquad [16]$$

since u satisfies the minimal surface equation. In sum, the form ω is closed and, given any X and Y at a point (x, y, z),

$$|\omega(X, Y)| \leq |X \times Y| \qquad [17]$$

where equality holds if and only if

$$X, Y \subset T_{(x,y,u(x,y))}\mathrm{Graph}_u \qquad [18]$$

Such a form ω is called a "calibration." From this, we have that if $\Sigma \subset \Omega \times \boldsymbol{R}$ is any other surface with $\partial\Sigma = \partial\,\mathrm{Graph}_u$, then by Stokes' theorem since ω is closed,

$$\mathrm{Area}(\mathrm{Graph}_u) = \int_{\mathrm{Graph}_u} \omega = \int_\Sigma \omega \leq \mathrm{Area}(\Sigma) \qquad [19]$$

This shows that Graph_u is area minimizing among all surfaces in the cylinder and with the same boundary. If the domain Ω is convex, the minimal graph is absolutely area minimizing. To see this, observe first that if Ω is convex, then so is $\Omega \times \boldsymbol{R}$ and hence the nearest point projection $P: \boldsymbol{R}^3 \to \Omega \times \boldsymbol{R}$ is a distance nonincreasing Lipschitz map that is equal to the identity on $\Omega \times \boldsymbol{R}$. If $\Sigma \subset \boldsymbol{R}^3$ is any other surface with $\partial\Sigma = \partial\,\mathrm{Graph}_u$, then $\Sigma' = P(\Sigma)$ has $\mathrm{Area}(\Sigma') \leq \mathrm{Area}(\Sigma)$. Applying [19] to Σ', we see that $\mathrm{Area}(\mathrm{Graph}_u) \leq \mathrm{Area}(\Sigma')$ and the claim follows.

If $\Omega \subset \boldsymbol{R}^2$ contains a ball of radius r, then, since $\partial B_r \cap \mathrm{Graph}_u$ divides ∂B_r into two components at least one of which has area at most equal to $(\mathrm{Area}(S^2)/2)r^2$, we get from [19] the crude estimate

$$\mathrm{Area}(B_r \cap \mathrm{Graph}_u) \leq \frac{\mathrm{Area}(S^2)}{2} r^2 \qquad [20]$$

When the domain Ω is convex, it is not hard to see that the minimal graph is absolutely area minimizing.

Very similar calculations to the ones above show that if $\Omega \subset \boldsymbol{R}^{n-1}$ and $u: \Omega \to \boldsymbol{R}$ is a C^2 function, then the graph of u is a critical point for the area functional if and only if u satisfies [14]. Moreover, as in [19], the graph of u is actually area minimizing. Consequently, as in [20], if Ω contains a ball of radius r, then

$$\mathrm{Vol}(B_r \cap \mathrm{Graph}_u) \leq \frac{\mathrm{Vol}(S^{n-1})}{2} r^{n-1} \qquad [21]$$

The Maximum Principle

The first variation formula, [2], showed that a smooth submanifold is a critical point for area if and only if the mean curvature vanishes. We will next derive the weak form of the first variation formula which is the basic tool for working with "weak solutions" (typically, stationary varifolds). Let X be a vector field on $\boldsymbol{R}^n$. We can write the divergence $\mathrm{div}_\Sigma X$ of X on Σ as

$$\begin{aligned}\mathrm{div}_\Sigma X &= \mathrm{div}_\Sigma X^{\mathrm{T}} + \mathrm{div}_\Sigma X^{\mathrm{N}} \\ &= \mathrm{div}_\Sigma X^{\mathrm{T}} + \langle X, \boldsymbol{H}\rangle \end{aligned} \qquad [22]$$

where X^{T} and X^{N} are the tangential and normal projections of X. In particular, we get that, for a minimal submanifold,

$$\mathrm{div}_\Sigma X = \mathrm{div}_\Sigma X^{\mathrm{T}} \qquad [23]$$

Moreover, from [22] and Stokes' theorem, we see that Σ is minimal if and only if for all vector fields X with compact support and vanishing on the boundary of Σ,

$$\int_\Sigma \mathrm{div}_\Sigma X = 0 \qquad [24]$$

The key point is that [24] makes sense as long as we can define the divergence on Σ. As a consequence of [24], we will show the following proposition:

Proposition 1 *$\Sigma^k \subset \boldsymbol{R}^n$ is minimal if and only if the restrictions of the coordinate functions of $\boldsymbol{R}^n$ to Σ are harmonic functions.*

Proof Let η be a smooth function on Σ with compact support and $\eta|\partial\Sigma = 0$, then

$$\int_\Sigma \langle \nabla_\Sigma \eta, \nabla_\Sigma x_i\rangle = \int_\Sigma \langle \nabla_\Sigma \eta, e_i\rangle = \int_\Sigma \mathrm{div}_\Sigma(\eta e_i) \qquad [25]$$

From this, the claim follows easily. □

Recall that if $\Xi \subset \boldsymbol{R}^n$ is a compact subset, then the smallest convex set containing Ξ (the convex hull, $\mathrm{Conv}(\Xi)$) is the intersection of all half-spaces containing Ξ. The maximum principle forces a compact minimal submanifold to lie in the convex hull of its boundary (this is the "convex hull property"):

Proposition 2 *If $\Sigma^k \subset \boldsymbol{R}^n$ is a compact minimal submanifold, then $\Sigma \subset \mathrm{Conv}(\partial\Sigma)$.*

Proof A half-space $H \subset \mathbf{R}^n$ can be written as

$$H = \{x \in \mathbf{R}^n | \langle x, e \rangle \leq a\} \qquad [26]$$

for a vector $e \in S^{n-1}$ and constant $a \in \mathbf{R}$. By Proposition 1, the function $u(x) = \langle e, x \rangle$ is harmonic on Σ and hence attains its maximum on $\partial\Sigma$ by the maximum principle. □

Another application of [23], with a different choice of vector field X, gives that for a k-dimensional minimal submanifold Σ

$$\Delta_\Sigma |x - x_0|^2 = 2\,\mathrm{div}_\Sigma(x - x_0) = 2k \qquad [27]$$

Later, we will see that this formula plays a crucial role in the monotonicity formula for minimal submanifolds.

The argument in the proof of the convex hull property can be rephrased as saying that as we translate a hyperplane towards a minimal surface, the first point of contact must be on the boundary. When Σ is a hypersurface, this is a special case of the strong maximum principle for minimal surfaces:

Lemma 1 *Let $\Omega \subset \mathbf{R}^{n-1}$ be an open connected neighborhood of the origin. If $u_1, u_2 : \Omega \to \mathbf{R}$ are solutions of the minimal surface equation with $u_1 \leq u_2$ and $u_1(0) = u_2(0)$, then $u_1 \equiv u_2$.*

Since any smooth hypersurface is locally a graph over a hyperplane, Lemma 1 gives a maximum principle for smooth minimal hypersurfaces.

Thus far, the examples of minimal submanifolds have all been smooth. The simplest nonsmooth example is given by a pair of planes intersecting transversely along a line. To get an example that is not even immersed, one can take three half-planes meeting along a line with an angle of $2\pi/3$ between each adjacent pair.

Monotonicity and the Mean-Value Inequality

Monotonicity formulas and mean-value inequalities play a fundamental role in many areas of geometric analysis.

Proposition 3 *Suppose that $\Sigma^k \subset \mathbf{R}^n$ is a minimal submanifold and $x_0 \in \mathbf{R}^n$; then for all $0 < s < t$,*

$$t^{-k}\,\mathrm{Vol}(B_t(x_0) \cap \Sigma) - s^{-k}\,\mathrm{Vol}(B_s(x_0) \cap \Sigma) = \int_{(B_t(x_0)\setminus B_s(x_0))\cap\Sigma} \frac{|(x - x_0)^N|^2}{|x - x_0|^{k+2}} \qquad [28]$$

Notice that $(x - x_0)^N$ vanishes precisely when Σ is conical about x_0, that is, when Σ is invariant under dilations about x_0. As a corollary, we get the following:

Corollary 1 *Suppose that $\Sigma^k \subset \mathbf{R}^n$ is a minimal submanifold and $x_0 \in \mathbf{R}^n$; then the function*

$$\Theta_{x_0}(s) = \frac{\mathrm{Vol}(B_s(x_0) \cap \Sigma)}{\mathrm{Vol}(B_s \subset \mathbf{R}^k)} \qquad [29]$$

is a nondecreasing function of s. Moreover, $\Theta_{x_0}(s)$ is constant in s if and only if Σ is conical about x_0.

Of course, if x_0 is a smooth point of Σ, then $\lim_{s\to 0} \Theta_{x_0}(s) = 1$. We will later see that the converse is also true; this will be a consequence of the Allard regularity theorem.

The monotonicity of area is a very useful tool in the regularity theory for minimal surfaces – at least when there is some *a priori* area bound. For instance, this monotonicity and a compactness argument allow one to reduce many regularity questions to questions about minimal cones (this was a key observation of W Fleming in his work on the Bernstein problem; see the section "The theorems of Bernstein and Bers").

Arguing as in Proposition 3, we get a weighted monotonicity:

Proposition 4 *If $\Sigma^k \subset \mathbf{R}^n$ is a minimal submanifold, $x_0 \in \mathbf{R}^n$, and f is a function on Σ, then*

$$\begin{aligned} t^{-k}\int_{B_t(x_0)\cap\Sigma} f - s^{-k}\int_{B_s(x_0)\cap\Sigma} f &= \int_{(B_t(x_0)\setminus B_s(x_0))\cap\Sigma} f\frac{|(x - x_0)^N|^2}{|x - x_0|^{k+2}} + \frac{1}{2}\int_s^t \tau^{-k-1} \\ &\quad \times \int_{B_\tau(x_0)\cap\Sigma} (\tau^2 - |x - x_0|^2)\Delta_\Sigma f\, d\tau \end{aligned} \qquad [30]$$

We get immediately the following mean-value inequality for the special case of non-negative subharmonic functions:

Corollary 2 *Suppose that $\Sigma^k \subset \mathbf{R}^n$ is a minimal submanifold, $x_0 \in \mathbf{R}^n$, and f is a non-negative subharmonic function on Σ; then*

$$s^{-k}\int_{B_s(x_0)\cap\Sigma} f \qquad [31]$$

is a nondecreasing function of s. In particular, if $x_0 \in \Sigma$, then for all $s > 0$,

$$f(x_0) \leq \frac{\int_{B_s(x_0)\cap\Sigma} f}{\mathrm{Vol}(B_s \subset \mathbf{R}^k)} \qquad [32]$$

Rado's Theorem

One of the most basic questions is what does the boundary $\partial\Sigma$ tell us about a compact minimal submanifold Σ? We have already seen that Σ must lie in the convex hull of $\partial\Sigma$, but there are many other theorems of this nature. One of the first theorems is a beautiful result of Rado which says that if $\partial\Sigma$ is a graph over the boundary of a convex set in $\mathbf{R}^2$, then Σ is also graph (and hence embedded). The proof of this uses basic properties of nodal lines for harmonic functions.

Theorem 1 *Suppose that $\Omega \subset \mathbf{R}^2$ is a convex subset and $\sigma \subset \mathbf{R}^3$ is a simple closed curve which is graphical over $\partial\Omega$. Then any minimal disk $\Sigma \subset \mathbf{R}^3$ with $\partial\Sigma = \sigma$ must be graphical over Ω and hence unique by the maximum principle.*

Proof (Sketch). The proof is by contradiction, so suppose that Σ is such a minimal disk and $x \in \Sigma$ is a point where the tangent plane to Σ is vertical. Consequently, there exists $(a, b) \neq (0, 0)$ such that

$$\nabla_\Sigma(ax_1 + bx_2)(x) = 0 \qquad [33]$$

By Proposition 1, $ax_1 + bx_2$ is harmonic on Σ (since it is a linear combination of coordinate functions). The local structure of nodal sets of harmonic functions (see, e.g., Colding and Minicozzi II (1999)) then gives that the level set

$$\{y \in \Sigma | ax_1 + bx_2(y) = ax_1 + bx_2(x)\} \qquad [34]$$

has a singularity at x where at least four different curves meet. If two of these nodal curves were to meet again, then there would be a closed nodal curve which must bound a disk (since Σ is a disk). By the maximum principle, $ax_1 + bx_2$ would have to be constant on this disk and hence constant on Σ by unique continuation. This would imply that $\sigma = \partial\Sigma$ is contained in the plane given by [34]. Since this is impossible, we conclude that all of these curves go to the boundary without intersecting again.

In other words, the plane in $\mathbf{R}^3$ given by [34] intersects σ in at least four points. However, since $\Omega \subset \mathbf{R}^2$ is convex, $\partial\Omega$ intersects the line given by [34] in exactly two points. Finally, since σ is graphical over $\partial\Omega$, σ intersects the plane in $\mathbf{R}^3$ given by [34] in exactly two points, which gives the desired contradiction. □

The Theorems of Bernstein and Bers

A classical theorem of S Bernstein from 1916 says that entire (i.e., defined over all of $\mathbf{R}^2$) minimal graphs are planes. This remarkable theorem of Bernstein was one of the first illustrations of the fact that the solutions to a nonlinear PDE, like the minimal surface equation, can behave quite differently from solutions to a linear equation.

Theorem 2 *If $u : \mathbf{R}^2 \to \mathbf{R}$ is an entire solution to the minimal surface equation, then u is an affine function.*

Proof (Sketch). We will show that the curvature of the graph vanishes identically; this implies that the unit normal is constant and, hence, the graph must be a plane. The proof follows by combining two facts. First, the area estimate for graphs [20] gives

$$\operatorname{Area}(B_r \cap \operatorname{Graph}_u) \leq 2\pi r^2 \qquad [35]$$

This quadratic area growth allows one to construct a sequence of non-negative logarithmic cutoff functions ϕ_j defined on the graph with $\phi_j \to 1$ everywhere and

$$\lim_{j\to\infty} \int_{\operatorname{Graph}_u} |\nabla\phi_j|^2 = 0 \qquad [36]$$

Moreover, since graphs are area minimizing, they must be stable. We can therefore use ϕ_j in the stability inequality [7] to get

$$\int_{\operatorname{Graph}_u} \phi_j^2 |A|^2 \leq \int_{\operatorname{Graph}_u} |\nabla\phi_j|^2 \qquad [37]$$

Combining these gives that $|A|^2$ is zero, as desired. □

Rather surprisingly, this result very much depended on the dimension. The combined efforts of E De Giorgi, F J Almgren Jr., and J Simons finally gave:

Theorem 3 *If $u : \mathbf{R}^{n-1} \to \mathbf{R}$ is an entire solution to the minimal surface equation and $n \leq 8$, then u is an affine function.*

However, in 1969, E Bombieri, De Giorgi, and E Giusti constructed entire nonaffine solutions to the minimal surface equation on $\mathbf{R}^8$ and an area-minimizing singular cone in $\mathbf{R}^8$. In fact, they showed that for $m \geq 4$, the cones

$$C_m = \{(x_1, \ldots, x_{2m}) \mid x_1^2 + \cdots + x_m^2 = x_{m+1}^2 + \cdots + x_{2m}^2\} \subset \mathbf{R}^{2m} \qquad [38]$$

are area minimizing (and obviously singular at the origin).

In contrast to the entire case, exterior solutions of the minimal graph equation, that is, solutions

on $R^2 \setminus B_1$, are much more plentiful. In this case, L Bers proved that ∇u actually has an asymptotic limit:

Theorem 4 *If u is a C^2 solution to the minimal surface equation on $R^2 \setminus B_1$, then ∇u has a limit at infinity (i.e., there is an asymptotic tangent plane).*

Bers' theorem was extended to higher dimensions by L Simon:

Theorem 5 *If u is a C^2 solution to the minimal surface equation on $R^n \setminus B_1$, then either*

(i) *$|\nabla u|$ is bounded and ∇u has a limit at infinity or*
(ii) *all tangent cones at infinity are of the form $\Sigma \times R$ where Σ is singular.*

Bernstein's theorem has had many other interesting generalizations, some of which will be discussed later.

Simons Inequality

In this section, we recall a very useful differential inequality for the Laplacian of the norm squared of the second fundamental form of a minimal hypersurface Σ in R^n and illustrate its role in *a priori* estimates. This inequality, originally due to J Simons, is:

Lemma 2 *If $\Sigma^{n-1} \subset R^n$ is a minimal hypersurface, then*

$$\Delta_\Sigma |A|^2 = -2|A|^4 + 2|\nabla_\Sigma A|^2 \geq -2|A|^4 \qquad [39]$$

An inequality of the type [39] on its own does not lead to pointwise bounds on $|A|^2$ because of the nonlinearity. However, it does lead to estimates if a "scale-invariant energy" is small. For example, H Choi and Schoen used [39] to prove:

Theorem 6 *There exists $\epsilon > 0$ so that if $0 \in \Sigma \subset B_r(0)$ with $\partial\Sigma \subset \partial B_r(0)$ is a minimal surface with*

$$\int |A|^2 \leq \epsilon \qquad [40]$$

then

$$|A|^2(0) \leq r^{-2} \qquad [41]$$

Heinz's Curvature Estimate for Graphs

One of the key themes in minimal surface theory is the usefulness of *a priori* estimates. A basic example is the curvature estimate of E Heinz for graphs. Heinz's estimate gives an effective version of the Bernstein's theorem; namely, letting the radius r_0 go to infinity in [42] implies that $|A|$ vanishes, thus giving Bernstein's theorem.

Theorem 7 *If $D_{r_0} \subset R^2$ and $u: D_{r_0} \to R$ satisfies the minimal surface equation, then for $\Sigma = Graph_u$ and $0 < \sigma \leq r_0$*

$$\sigma^2 \sup_{D_{r_0-\sigma}} |A|^2 \leq C \qquad [42]$$

Proof (Sketch). Observe first that it suffices to prove the estimate for $\sigma = r_0$, that is, to show that

$$|A|^2(0, u(0)) \leq C r_0^{-2} \qquad [43]$$

Recall that minimal graphs are automatically stable. As in the proof of Theorem 2, the area estimate for graphs [20] allows us to use a logarithmic cutoff function in the stability inequality [7] to get that

$$\int_{B_{r_1} \cap \mathrm{Graph}_u} |A|^2 \leq \frac{C}{\log(r_0/r_1)} \qquad [44]$$

Taking r_0/r_1 sufficiently large, we can then apply Theorem 6 to get [43]. □

Embedded Minimal Disks with Area Bounds

In the early 1980s, Schoen and Simon extended the theorem of Bernstein to complete simply connected embedded minimal surfaces in R^3 with quadratic area growth. A surface Σ is said to have quadratic area growth if for all $r > 0$, the intersection of the surface with the ball in R^3 of radius r and center at the origin is bounded by Cr^2 for a fixed constant C independent of r.

Theorem 8 *Let $0 \in \Sigma^2 \subset B_{r_0} = B_{r_0}(x) \subset R^3$ be an embedded simply connected minimal surface with $\partial\Sigma \subset \partial B_{r_0}$. If $\mu > 0$ and either*

$$\mathrm{Area}(\Sigma) \leq \mu r_0^2 \quad or \quad \int_\Sigma |A|^2 \leq \mu \qquad [45]$$

then for the connected component Σ' of $B_{r_0/2}(x_0) \cap \Sigma$ with $0 \in \Sigma'$ we have

$$\sup_{\Sigma'} |A|^2 \leq C r_0^{-2} \qquad [46]$$

for some $C = C(\mu)$.

The result of Schoen–Simon was generalized by Colding–Minicozzi to quadratic area growth for intrinsic balls (this generalization played an important role in analyzing the local structure of embedded minimal surfaces):

Theorem 9 *Given a constant C_I, there exists C_P so that if $\mathcal{B}_{2r_0} \subset \Sigma \subset R^3$ is an embedded minimal disk satisfying either*

$$\mathrm{Area}(\mathcal{B}_{2r_0}) \leq C_I r_0^2 \quad or \quad \int_{\mathcal{B}_{2r_0}} |A|^2 \leq C_I \qquad [47]$$

then

$$\sup_{\mathcal{B}_s} |A|^2 \leq C_P s^{-2} \qquad [48]$$

As an immediate consequence, letting $r_0 \to \infty$ gives Bernstein-type theorems for embedded simply connected minimal surfaces with either bounded density or finite total curvature. Note that Enneper's surface is simply connected but neither flat nor embedded; this shows that embeddedness is essential for these estimates. Similarly, the catenoid shows that the surface being simply connected is essential. The catenoid is the minimal surface in $\mathbf{R}^3$ given by

$$\{(\cosh s \cos t, \cosh s \sin t, s) | s, t \in \mathbf{R}\} \qquad [49]$$

Stable Minimal Surfaces

It turns out that stable minimal surfaces have *a priori* estimates. Since minimal graphs are stable, the estimates for stable surfaces can be thought of as generalizations of the earlier estimates for graphs. These estimates have been widely applied and are particularly useful when combined with existence results for stable surfaces (such as the solution of the Plateau problem). The starting point for these estimates is that, as we saw in [4], stable minimal surfaces satisfy the stability inequality

$$\int |A|^2 \phi^2 \leq \int |\nabla \phi|^2 \qquad [50]$$

We will mention two such estimates. The first is R Schoen's curvature estimate for stable surfaces:

Theorem 10 *There exists a constant C so that if $\Sigma \subset \mathbf{R}^3$ is an immersed stable minimal surface with trivial normal bundle and $\mathcal{B}_{r_0} \subset \Sigma \backslash \partial \Sigma$, then*

$$\sup_{\mathcal{B}_{r_0 - \sigma}} |A|^2 \leq C \sigma^{-2} \qquad [51]$$

The second is an estimate for the area and total curvature of a stable surface is due to Colding–Minicozzi; for simplicity, we will state only the area estimate:

Theorem 11 *If $\Sigma \subset \mathbf{R}^3$ is an immersed stable minimal surface with trivial normal bundle and $\mathcal{B}_{r_0} \subset \Sigma \backslash \partial \Sigma$, then*

$$\text{Area}(\mathcal{B}_{r_0}) \leq 4\pi r_0^2 / 3 \qquad [52]$$

As mentioned, we can use [52] to bound the energy of a cutoff function in the stability inequality and, thus, bound the total curvature of sub-balls. Combining this with the curvature estimate of Theorem 6 gives Theorem 10. Note that the bound [53] is surprisingly sharp; even when Σ is a plane, the area is πr_0^2.

Regularity Theory

In this section, we survey some of the key ideas in classical regularity theory, such as the role of monotonicity, scaling, ϵ-regularity theorems (such as Allard's theorem) and tangent cone analysis (such as Almgren's refinement of Federer's dimension reducing). We refer to the book by Morgan (1995) for a more detailed overview and a general introduction to geometric measure theory.

The starting point for all of this is the monotonicity of volume for a minimal k-dimensional submanifold Σ. Namely, Corollary [1] gives that the density

$$\Theta_{x_0}(s) = \frac{\text{Vol}(B_s(x_0) \cap \Sigma)}{\text{Vol}(B_s \subset \mathbf{R}^k)} \qquad [53]$$

is a monotone nondecreasing function of s. Consequently, we can define the density Θ_{x_0} at the point x_0 to be the limit as $s \to 0$ of $\Theta_{x_0}(s)$. It also follows easily from monotonicity that the density is semicontinuous as a function of x_0.

ϵ-Regularity and the Singular Set

An ϵ-regularity theorem is a theorem giving that a weak (or generalized) solution is actually smooth at a point if a scale-invariant energy is small enough there. The standard example is the Allard regularity theorem:

Theorem 12 *There exists $\delta(k, n) > 0$ such that if $\Sigma \subset \mathbf{R}^n$ is a k-rectifiable stationary varifold (with density at least one a.e.), $x_0 \in \Sigma$, and*

$$\Theta_{x_0} = \lim_{r \to 0} \frac{\text{Vol}(B_r(x_0) \cap \Sigma)}{\text{Vol}(B_r \subset \mathbf{R}^k)} < 1 + \delta \qquad [54]$$

then Σ is smooth in a neighborhood of x_0.

Similarly, the small total curvature estimate of Theorem 6 may be thought of as an ϵ-regularity theorem; in this case, the scale-invariant energy is $\int |A|^2$.

As an application of the ϵ-regularity theorem, Theorem [12], we can define the singular set $\mathcal{S}$ of Σ by

$$\mathcal{S} = \{x \in \Sigma | \Theta_x \geq 1 + \delta\} \qquad [55]$$

It follows immediately from the semicontinuity of the density that $\mathcal{S}$ is closed. In order to bound the size of the singular set (e.g., the Hausdorff measure), one combines the ϵ-regularity with simple covering arguments.

This preliminary analysis of the singular set can be refined by doing a so-called tangent cone analysis.

Tangent Cone Analysis

It is not hard to see that scaling preserves the space of minimal submanifolds of $\boldsymbol{R}^n$. Namely, if Σ is minimal, then so is

$$\Sigma_{y,\lambda} = \{y + \lambda^{-1}(x - y) | x \in \Sigma\} \qquad [56]$$

(To see this, simply note that this scaling multiplies the principal curvatures by λ.) Suppose now that we fix the point y and take a sequence $\lambda_j \to 0$. The monotonicity formula bounds the density of the rescaled solution, allowing us to extract a convergent subsequence and limit. This limit, which is called a "tangent cone" at y, achieves equality in the monotonicity formula and, hence, must be homogeneous (i.e., invariant under dilations about y).

The usefulness of tangent cone analysis in regularity theory is based on two key facts. For simplicity, we illustrate these when $\Sigma \subset \boldsymbol{R}^n$ is an area-minimizing hypersurface. First, if any tangent cone at y is a hyperplane $\boldsymbol{R}^{n-1}$, then Σ is smooth in a neighborhood of y. This follows easily from the Allard regularity theorem since the density at y of the tangent cone is the same as the density at y of Σ. The second key fact, known as "dimension reducing," is due to Almgren and is a refinement of an argument of Federer. To state this, we first stratify the singular set $\mathcal{S}$ of Σ into subsets

$$\mathcal{S}_0 \subset \mathcal{S}_1 \subset \cdots \subset \mathcal{S}_{n-2} \qquad [57]$$

where we define $\mathcal{S}_i$ to be the set of points $y \in \mathcal{S}$ so that any linear space contained in any tangent cone at y has dimension at most i. (Note that $\mathcal{S}_{n-1} = \emptyset$ by Allard's theorem.) The dimension reducing argument then gives that

$$\dim(\mathcal{S}_i) \leq i \qquad [58]$$

where dimension means the Hausdorff dimension. In particular, the solution of the Bernstein problem then gives codimension-7 regularity of Σ, that is, $\dim(\mathcal{S}) \leq n - 8$.

Part 2. Constructing Minimal Surfaces

Thus far, we have mainly dealt with regularity and *a priori* estimates but have ignored questions of existence. In this part, we survey some of the most useful existence results for minimal surfaces. The following section gives an overview of the classical Plateau problem. Next, we recall the classical Weierstrass representation, including a few modern applications, and the Kapouleas desingularization method. Then we deal with producing area-minimizing surfaces and questions of embeddedness. Finally, we recall the min–max construction for producing unstable minimal surfaces and, in particular, doing so while controlling the topology and guaranteeing embeddedness.

The Plateau Problem

The following fundamental existence problem for minimal surfaces is known as the Plateau problem: given a closed curve Γ, find a minimal surface with boundary Γ. There are various solutions to this problem depending on the exact definition of a surface (parametrized disk, integral current, $\boldsymbol{Z}_2$ current, or rectifiable varifold). We shall consider the version of the Plateau problem for parametrized disks; this was solved independently by J Douglas and T Rado. The generalization to Riemannian manifolds is due to C B Morrey.

Theorem 13 *Let $\Gamma \subset \boldsymbol{R}^3$ be a piecewise C^1 closed Jordan curve. Then there exists a piecewise C^1 map u from $D \subset \boldsymbol{R}^2$ to $\boldsymbol{R}^3$ with $u(\partial D) \subset \Gamma$ such that the image minimizes area among all disks with boundary Γ.*

The solution u to the Plateau problem above can easily be seen to be a branched conformal immersion. R Osserman proved that u does not have true interior branch points; subsequently, R Gulliver and W Alt showed that u cannot have false branch points either.

Furthermore, the solution u is as smooth as the boundary curve, even up to the boundary. A very general version of this boundary regularity was proved by S Hildebrandt; for the case of surfaces in $\boldsymbol{R}^3$, recall the following result of J C C Nitsche:

Theorem 14 *If Γ is a regular Jordan curve of class $C^{k,\alpha}$ where $k \geq 1$ and $0 < \alpha < 1$, then a solution u of the Plateau problem is $C^{k,\alpha}$ on all of $\bar{D}$.*

The Weierstrass Representation

The classical Weierstrass representation (see Osserman (1986)) takes holomorphic data (a Riemann surface, a meromorphic function, and a holomorphic 1-form) and associates a minimal surface in $\boldsymbol{R}^3$. To be precise, given a Riemann surface Ω, a meromorphic function g on Ω, and a holomorphic 1-form ϕ on Ω, then we

get a (branched) conformal minimal immersion $F:\Omega \to \mathbf{R}^3$ by

$$F(z) = \mathrm{Re} \int_{\zeta \in \gamma_{z_0,z}} \left(\frac{1}{2}(g^{-1}(\zeta) - g(\zeta)), \right. \\ \left. \frac{\mathrm{i}}{2}(g^{-1}(\zeta) + g(\zeta)), 1 \right) \phi(\zeta) \quad [59]$$

Here, $z_0 \in \Omega$ is a fixed base point and the integration is along a path $\gamma_{z_0,z}$ from z_0 to z. The choice of z_0 changes F by adding a constant. In general, the map F may depend on the choice of path (and hence may not be well defined); this is known as "the period problem." However, when g has no zeros or poles and Ω is simply connected, then $F(z)$ does not depend on the choice of path $\gamma_{z_0,z}$.

Two standard constructions of minimal surfaces from Weierstrass data are

$$g(z) = z,\ \phi(z) = \mathrm{d}z/z,\ \Omega = \mathbf{C}\backslash\{0\} \\ \text{giving a catenoid} \quad [60]$$

$$g(z) = \mathrm{e}^{\mathrm{i}z},\ \phi(z) = \mathrm{d}z,\ \Omega = \mathbf{C} \text{ giving a helicoid} \quad [61]$$

The Weierstrass representation is particularly useful for constructing immersed minimal surfaces. Typically, it is rather difficult to prove that the resulting immersion is an embedding (i.e., is 1–1), although there are some interesting cases where this can be done. For the first modern example, D Hoffman and Meeks proved that the surface constructed by Costa was embedded; this was the first new complete finite topology properly embedded minimal surface discovered since the classical catenoid, helicoid, and plane. This led to the discovery of many more such surfaces (see Rosenberg (1992) for more discussion).

Area-Minimizing Surfaces

Perhaps the most natural way to construct minimal surfaces is to look for ones which minimize area, for example, with fixed boundary, or in a homotopy class, etc. This has the advantage that often it is possible to show that the resulting surface is embedded. We mention a few results along these lines.

The first embeddedness result, due to Meeks and Yau, shows that if the boundary curve is embedded and lies on the boundary of a smooth mean convex set (and it is null-homotopic in this set), then it bounds an embedded least area disk.

Theorem 15 (Meeks III and Yau 1982). *Let M^3 be a compact Riemannian 3-manifold whose boundary is mean convex and let γ be a simple closed curve in ∂M which is null-homotopic in M; then γ is bounded by a least area disk and any such least area disk is properly embedded.*

Note that some restriction on the boundary curve γ is certainly necessary. For instance, if the boundary curve was knotted (e.g., the trefoil), then it could not be spanned by any embedded disk (minimal or otherwise). Prior to the work of Meeks and Yau, embeddedness was known for extremal boundary curves in $\mathbf{R}^3$ with small total curvature by the work of R Gulliver and J Spruck.

If we instead fix a homotopy class of maps, then the two fundamental existence results are due to Sacks–Uhlenbeck and Schoen–Yau (with embeddedness proved by Meeks–Yau and Freedman–Hass–Scott, respectively):

Theorem 16 *Given M^3, there exist conformal (stable) minimal immersions $u_1, \ldots, u_m : S^2 \to M$ which generate $\pi_2(M)$ as a $\mathbf{Z}[\pi_1(M)]$ module. Furthermore,*

(i) *if* $u : S^2 \to M$ *and* $[u]_{\pi_2} \neq 0$, *then* $\mathrm{Area}(u) \geq \min_i \mathrm{Area}(u_i)$,
(ii) *each u_i is either an embedding or a 2–1 map onto an embedded two-sided RP^2.*

Theorem 17 *If Σ^2 is a closed surface with genus $g > 0$ and $i_0 : \Sigma \to M^3$ is an embedding which induces an injective map on π_1, then there is a least area embedding with the same action on π_1.*

The Min–Max Construction of Minimal Surfaces

Variational arguments can also be used to construct higher index (i.e., nonminimizing) minimal surfaces using the topology of the space of surfaces. There are two basic approaches:

1. Applying Morse theory to the energy functional on the space of maps from a fixed surface Σ to M.
2. Doing a min–max argument over families of (topologically nontrivial) sweep-outs of M.

The first approach has the advantage that the topological type of the minimal surface is easily fixed; however, the second approach has been more successful at producing embedded minimal surfaces. We will highlight a few key results below but refer to Colding and De Lellis (2003) for a thorough treatment.

Unfortunately, one cannot directly apply Morse theory to the energy functional on the space of maps from a fixed surface because of a lack of compactness (the Palais–Smale condition C does not hold).

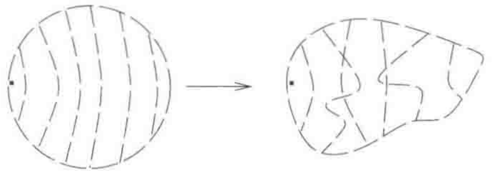


Figure 1 A one-parameter family of curves on a 2-sphere which induces a map $F: \mathbf{S}^2 \to \mathbf{S}^2$ of degree 1. First published in Surveys in Differential Geometry, volume IX, in 2004, published by International Press.

To get around this difficulty, Sacks–Uhlenbeck introduce a family of perturbed energy functionals which do satisfy condition C and then obtain minimal surfaces as limits of critical points for the perturbed problems:

Theorem 18 *If $\pi_k(M) \neq 0$ for some $k > 1$, then there exists a branched immersed minimal 2-sphere in M (for any metric).*

The basic idea of constructing minimal surfaces via min–max arguments and sweep-outs goes back to Birkhoff, who developed it to construct simple closed geodesics on spheres. In particular, when M is a topological 2-sphere, we can find a one-parameter family of curves starting and ending at point curves so that the induced map $F: S^2 \to S^2$ (see **Figure 1**) has nonzero degree. The min–max argument produces a nontrivial closed geodesic of length less than or equal to the longest curve in the initial one-parameter family. A curve-shortening argument gives that the geodesic obtained in this way is simple.

J Pitts applied a similar argument and geometric measure theory to get that every closed Riemannian 3-manifold has an embedded minimal surface (his argument was for dimensions up to seven), but he did not estimate the genus of the resulting surface. Finally, F Smith (under the direction of L Simon) proved (see Colding and De Lellis (2003)):

Theorem 19 *Every metric on a topological 3-sphere M admits an embedded minimal 2-sphere.*

The main new contribution of Smith was to control the topological type of the resulting minimal surface while keeping it embedded.

Part 3. Some Applications of Minimal Surfaces

In this part, we discuss very briefly a few applications of minimal surfaces. As mentioned in the introduction, there are many to choose from and we have selected just a few.

The Positive-Mass Theorem

The (Riemannian version of the) positive-mass theorem states that an asymptotically flat 3-manifold M with non-negative scalar curvature must have positive mass. The Riemannian manifold M here arises as a maximal spacelike slice in a $(3+1)$-dimensional spacetime solution of Einstein's equations.

The asymptotic flatness of M arises because the spacetime models an isolated gravitational system and hence is a perturbation of the vacuum solution outside a large compact set. To make this precise, suppose for simplicity that M has only one end; M is then said to be asymptotically flat if there is a compact set $\Omega \subset M$ so that $M \backslash \Omega$ is diffeomorphic to $\mathbf{R}^3 \backslash B_R(0)$ and the metric on $M \backslash \Omega$ can be written as

$$g_{ij} = \left(1 + \frac{\mathcal{M}}{2|x|}\right)^4 \delta_{ij} + p_{ij} \qquad [62]$$

where

$$|x|^2 |p_{ij}| + |x|^3 |Dp_{ij}| + |x|^4 |D^2 p_{ij}| \leq C \qquad [63]$$

The constant $\mathcal{M}$ is the so-called mass of M. Observe that the metric g_{ij} is a perturbation of the metric on a constant-time slice in the Schwarzschild spacetime of mass $\mathcal{M}$; that is to say, the Schwarzschild metric has $p_{ij} \equiv 0$.

A tensor h is said to be $O(|x|^{-p})$ if $|x|^p |h| + |x|^{p+1} |Dh| \leq C$. For example, an easy calculation shows that

$$\begin{aligned} g_{ij} &= (1 + 2\mathcal{M}/|x|)\, \delta_{ij} + O(|x|^{-2}) \\ \sqrt{g} &\equiv \sqrt{\det g_{ij}} = 1 + 3\mathcal{M}|x|^{-1} + O(|x|^{-2}) \end{aligned} \qquad [64]$$

The positive-mass theorem states that the mass $\mathcal{M}$ of such an M must be non-negative:

Theorem 20 (Schoen and Yau 1979). *With M as above, $\mathcal{M} \geq 0$.*

There is a rigidity theorem as well which states that the mass vanishes only when M is isometric to $\mathbf{R}^3$:

Theorem 21 (Schoen and Yau 1979). *If $|\nabla^3 p_{ij}| = O(|x|^{-5})$ and $\mathcal{M} = 0$ in* Theorem 20, *then M is isometric to* $\mathbf{R}^3$.

We will give a very brief overview of the proof of Theorem 20, showing in the process where minimal surfaces appear.

Proof (Sketch). The argument will be by contradiction, so suppose that the mass is negative. It is not hard to prove that the slab between two parallel

planes is mean convex. That is, we have the following:

Lemma 3 *If $\mathcal{M} < 0$ and M is asymptotically flat, then there exist $R_0, h > 0$ so that for $r > R_0$ the sets*

$$C_r = \{|x|^2 \leq r^2, -h \leq x_3 \leq h\} \qquad [65]$$

have strictly mean-convex boundary.

Since the compact set C_r is mean convex, we can solve the Plateau problem to get an area-minimizing (and hence stable) surface $\Gamma_r \subset C_r$ with boundary

$$\partial\Gamma_r = \{|x|^2 = r^2, x_3 = h\} \qquad [66]$$

Using the disk $\{|x|^2 \leq r^2, x_3 = h\}$ as a comparison surface, we get uniform local area bounds for any such Γ_r. Combining these local area bounds with the *a priori* curvature estimates for minimizing surfaces, we can take a sequence of r's going to infinity and find a subsequence of Γ_r's that converge to a complete area-minimizing surface

$$\Gamma \subset \{-h \leq x_3 \leq h\} \qquad [67]$$

Since Γ is pinched between the planes $\{x_3 = \pm h\}$, the estimates for minimizing surfaces implies that (outside a large compact set) Γ is a graph over the plane $\{x_3 = 0\}$ and hence has quadratic area growth and finite total curvature. Moreover, using the form of the metric g_{ij}, we see that $|\nabla u|$ decays like $|x|^{-1}$ and

$$\int_{\sigma_s} k_g = (2\pi s + O(1))(s^{-1} + O(s^{-2})) \\ = 2\pi + O(s^{-1}) \qquad [68]$$

where $\sigma_s = \{x_1^2 + x_2^2 = s^2\} \cap \Gamma$ and k_g is the geodesic curvature of σ_s (as a curve in Γ).

To get the contradiction, one combines stability of Γ with the positive scalar curvature of M to see that no such Γ could have existed. (M was assumed only to have non-negative scalar curvature. However, a "rounding off" argument shows that the metric on M can be perturbed to have positive scalar curvature outside of a compact set and still have negative mass.) Namely, substituting the Gauss equation into the stability inequality (this is the stability inequality in a general 3-manifold; see Colding and Minicozzi II (1999)) gives

$$\int_\Gamma (|A|^2/2 + \text{Scal}_M - K_\Sigma)\phi^2 \leq \int_\Gamma |\nabla\phi|^2 \qquad [69]$$

Since Γ has quadratic area growth, we can choose a sequence of (logarithmic) cutoff functions in [69] to get

$$0 < \int_\Sigma (|A|^2/2 + \text{Scal}_M) \leq \int_\Sigma K_\Sigma < \infty \qquad [70]$$

since K_Σ may not be positive, we also used that Γ has finite total curvature. Moreover, we used that Scal_M is positive outside a compact set to see that the first integral in [70] was positive. Finally, substituting [70] into the Gauss–Bonnet formula gives that $\int_{\sigma_s} k_g$ is strictly less than 2π for s large, contradicting [68].

Black holes

Another way that minimal surfaces enter into relativity is through black holes. Suppose that we have a three-dimensional time slice M in a $(3+1)$-dimensional spacetime. For simplicity, assume that M is totally geodesic and hence has non-negative scalar curvature. A closed surface Σ in M is said to be trapped if its mean curvature is everywhere negative with respect to its outward normal. Physically, this means that the surface emits an outward shell of light whose surface area is decreasing everywhere on the surface. The existence of a closed trapped surface implies the existence of a black hole in the spacetime.

Given a trapped surface, we can look for the outermost trapped surface containing it; this outermost surface is called an apparent horizon. It is not hard to see that an apparent horizon must be a minimal surface and, moreover, a barrier argument shows that it must be stable. Since M has non-negative scalar curvature, stability in turn implies that it must be diffeomorphic to a sphere. See, for instance, Bray (2002) for references to some results on black holes, horizons, etc.

Constant Mean Curvature Surfaces

At least since the time of Plateau, minimal surfaces have been used to model soap films. This is because the mean curvature of the surface models the surface tension and this is essentially the only force acting on a soap film. Soap bubbles, on other hand, enclose a volume and thus the pressure gives a second counterbalancing force. It follows easily that these two forces are in equilibrium when the surface has constant mean curvature (cmc).

For the same reason, cmc surfaces arise in the isoperimetric problem. Namely, a surface that minimizes surface area while enclosing a fixed volume must have cmc. It is not hard to see that such an isoperimetric surface in $\mathbf{R}^n$ must be a round sphere. There are two interesting partial converses to this. First, by a theorem of Hopf, any cmc 2-sphere in $\mathbf{R}^3$ must be round. Second, using the maximum principle ("the method of moving planes"), Alexandrov showed that any closed embedded cmc hypersurface in $\mathbf{R}^n$ must be a round sphere. It turned out, however, that not every closed immersed cmc surface is round. The

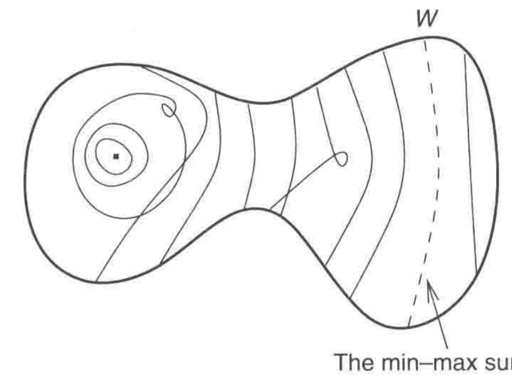


Figure 2 The sweep-out, the min–max surface, and the width *W*. First published in the *Journal of the American Mathematical Society* in 2005, published by the American Mathematical Society.

first examples were immersed cmc tori constructed by H Wente. Kapouleas constructed many new examples, including closed higher-genus cmc surfaces.

Many of the techniques developed for studying minimal surfaces generalize to general cmc surfaces.

Finite Extinction for Ricci Flow

We close this article by indicating how minimal surfaces can be used to show that on a homotopy 3-sphere the Ricci flow becomes extinct in finite time (see Colding and Minicozzi II (2005) and Perelman (2003) for details).

Let M^3 be a smooth closed orientable 3-manifold and let $g(t)$ be a one-parameter family of metrics on M evolving by the Ricci flow, so

$$\partial_t g = -2\mathrm{Ric}_{M_t} \qquad [71]$$

In an earlier section, we saw that there is a natural way of constructing minimal surfaces on many 3-manifolds and that comes from the min–max argument where the minimal of all maximal slices of sweep-outs is a minimal surface. The idea is then to look at how the area of this min–max surface changes under the flow. Geometrically, the area measures a kind of width of the 3-manifold and as we will see for certain 3-manifolds (those, like the 3-sphere, whose prime decomposition contains no aspherical factors), the area becomes zero in finite time corresponding to the solution becoming extinct in finite time.

Fix a continuous map $\beta: [0,1] \to C^0 \cap L_1^2(S^2, M)$ where $\beta(0)$ and $\beta(1)$ are constant maps so that β is in the nontrivial homotopy class $[\beta]$ (such β exists when M is a homotopy 3-sphere). We define the width $W = W(g, [\beta])$ by

$$W(g) = \min_{\gamma \in [\beta]} \max_{s \in [0,1]} \mathrm{Energy}(\gamma(s)) \qquad [72]$$

The next theorem gives an upper bound for the derivative of $W(g(t))$ under the Ricci flow which forces the solution $g(t)$ to become extinct in finite time.

Theorem 22 *Let M^3 be a homotopy 3-sphere equipped with a Riemannian metric $g = g(0)$. Under the Ricci flow, the width $W(g(t))$ satisfies*

$$\frac{\mathrm{d}}{\mathrm{d}t} W(g(t)) \le -4\pi + \frac{3}{4(t+C)} W(g(t)) \qquad [73]$$

in the sense of the limsup of forward difference quotients. Hence, $g(t)$ must become extinct in finite time.

The 4π in [73] comes from the Gauss–Bonnet theorem and the 3/4 comes from the bound on the minimum of the scalar curvature that the evolution equation implies. Both of these constants matter whereas the constant C depends on the initial metric and the actual value is not important.

To see that [73] implies finite extinction time, rewrite [73] as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(W(g(t))(t+C)^{-3/4}\right) \le -4\pi(t+C)^{-3/4} \qquad [74]$$

and integrate to get

$$(T+C)^{-3/4} W(g(T)) \le C^{-3/4} W(g(0)) - 16\pi\left[(T+C)^{1/4} - C^{1/4}\right] \qquad [75]$$

Since $W \ge 0$ by definition and the right-hand side of [75] would become negative for T sufficiently large, we get the claim.

As a corollary of this theorem we get finite extinction time for the Ricci flow.

Corollary 3 *Let M^3 be a homotopy 3-sphere equipped with a Riemannian metric $g = g(0)$. Under the Ricci flow $g(t)$ must become extinct in finite time.*

Acknowledgments

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See also: Black Hole Mechanics; Calibrated Geometry and Special Lagrangian Submanifolds; Geometric Analysis and General Relativity; Geometric Measure Theory; Leray–Schauder Theory and Mapping Degree; Ljusternik–Schnirelman Theory; Singularities of the Ricci Flow.

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Minimax Principle in the Calculus of Variations

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Introduction

When studying a functional f on an infinite-dimensional function space X, one is often interested in finding critical points which are not local minima. A simple yet powerful method to detect those critical points is the minimax method. The idea consists in detecting some complexity in the topology of X, or in the structure of the sublevels of f, to find a class Γ of subsets of X which somehow reveals such a topological complexity, and to show that the number

$$c := \inf_{\gamma \in \Gamma} \sup_{x \in \gamma} f(x)$$

is finite (even if the functional may be unbounded above and below). If the class Γ is positively invariant under the action of the negative-gradient flow of f, and if a suitable compactness assumption known as the Palais–Smale condition holds, c is proved to be a critical value of f. Quite remarkably, the minimax method also works when no topological complexity is present, but the negative-gradient flow of f exhibits some kind of rigidity.

In this article we shall describe these ideas, starting from the simplest minimax result, the "mountain-pass theorem." We will show how to apply the minimax method by discussing the existence question of solutions of a nonlinear elliptic boundary value problem, of closed geodesics on compact manifolds, and of closed characteristics on compact energy hypersurfaces.

The Mountain-Pass Theorem

Let us start by considering the following familiar fact. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a smooth coercive function (i.e., its sublevels have compact closure). If a sublevel $\{f < a\}$ is not connected – say $\{f < a\} = A \cup B$, with A, B disjoint open sets – then f has a critical point x at level

$$f(x) = c := \inf_{\gamma \in \Gamma} \max_{u \in \gamma} f(u) \geq a$$

where Γ is the class of all continuous curves in $\mathbb{R}^n$ with one end point in A and the other in B. More figuratively: if there are two valleys, then there must be a mountain pass. Let us examine a possible proof.

First notice that any curve in the class Γ will have to cross the level $\{f = a\}$, so $c \geq a$. If by contradiction c is not a critical value of f, by the compactness of the sublevels there is some $\epsilon > 0$ such that $|\nabla f| \geq \epsilon$ on $\{c - \epsilon \leq f \leq c + \epsilon\}$. Then the negative-gradient flow of f, that is, the solution of

$$\partial_t \phi(t, u) = -\nabla f(\phi(t, u)), \quad \phi(0, u) = u$$

pulls the sublevel $\{f \leq c+\epsilon\}$ down into the sublevel $\{f \leq c-\epsilon\}$ in finite time $2/\epsilon$. Indeed, if $\phi([0,t],u) \subset \{c-\epsilon \leq f \leq c+\epsilon\}$, then the inequalities

$$\begin{aligned} 2\epsilon &\geq f(u) - f(\phi(t,u)) \\ &= -\int_0^t \frac{\mathrm{d}}{\mathrm{d}s} f(\phi(s,u))\,\mathrm{d}s \\ &= \int_0^t |\nabla f(\phi(s,u))|^2\,\mathrm{d}s \geq \epsilon^2 t \end{aligned}$$

imply that $t \leq 2/\epsilon$. By definition of c, we can find a continuous curve $\gamma \in \Gamma$ which is contained in $\{f \leq c+\epsilon\}$. But then the curve $\gamma' := \phi(2/\epsilon, \gamma)$ still has one end point in A, the other one in B, and lies in $\{f \leq c-\epsilon\}$, contradicting the definition of c.

If we try to generalize this result to functions defined on an infinite-dimensional real Hilbert space H, we encounter difficulties due to lack of compactness. Indeed, a continuous function on an infinite-dimensional Hilbert space can never have compact sublevels (with respect to the norm topology). If we look back at the proof, we see that we have used coercivity to guarantee that if the level set $\{f = c\}$ contains no critical points, then ∇f is bounded away from zero on the strip $\{c-\epsilon \leq f \leq c+\epsilon\}$, for some small $\epsilon > 0$. A natural idea is then to replace the coercivity assumption by a condition implying the latter fact.

Definition Let $f : H \to \mathbb{R}$ be a continuously differentiable function on a real Hilbert space H. A sequence $(u_h) \subset H$ is said a Palais–Smale sequence if $f(u_h)$ is bounded and $Df(u_h)$ tends to zero. The function f is said to satisfy the Palais–Smale condition if every Palais–Smale sequence has a converging subsequence.

The Palais–Smale condition readily implies the statement above. Assuming also that f is twice continuously differentiable, the negative-gradient flow of f (a well-defined local flow because ∇f is continuously differentiable) pulls the sublevel $\{f \leq c+\epsilon\}$ down into $\{f \leq c-\epsilon\}$ in finite time. These observations lead to the following:

Theorem (Mountain pass). *Let f be a twice continuously differentiable function on a real Hilbert space H, satisfying the Palais–Smale condition. Assume that a sublevel $\{f < a\}$ is not connected, and let A, B be two disjoint open sets such that $A \cup B = \{f < a\}$. Then f has a critical point x at level*

$$f(x) = c := \inf_{\gamma \in \Gamma} \max_{u \in \gamma} f(u) \geq a$$

where Γ is the class of all continuous curves in H with one end point in A and the other one in B.

If we are even more ambitious, and we wish to consider functions defined on a real Banach space E, we also encounter the problem of not having a gradient vector field. Indeed, the differential of f at x, $Df(x)$, is an element of the dual space E^*, but in this case we have no inner product on E by which we can represent $Df(x)$ as the product by some vector of E. This problem can be overcome by the notion of a pseudogradient vector field. In fact, it can be proved that if f is continuously differentiable on E, then there exists a locally Lipschitz vector field V defined on the complement of the critical points of f, such that

$$\begin{aligned} &\|V(u)\| < \min\{\|Df(u)\|, 1\} \\ &Df(u)[V(u)] > \tfrac{1}{2}\min\{\|Df(u)\|, 1\}\|Df(u)\| \end{aligned}$$

In other words, even if there is no direction of steepest increase for f, we do have directions along which the increase of f is steep enough, and these directions can be selected in a locally Lipschitz way. Notice that pseudogradients are useful also in the case of a continuously differentiable function on a Hilbert space: in this case the gradient of f is just continuous, so it does not generate a flow. The Palais–Smale condition, as stated above, makes perfect sense on the Banach space E (with the only difference that now $Df(u_h)$ tends to zero in the dual norm of E^*), and the mountain-pass theorem holds for functions of class C^1 on a Banach space.

Actually, the fact that the domain of f has a vector structure is not relevant in this statement, and the mountain-pass theorem holds also for functions defined on connected infinite-dimensional manifolds. Since the essential feature is to dispose of a pseudogradient vector field, the right level of generality is to consider a Banach manifold M (i.e., a manifold modeled on a Banach space) endowed with a complete Finsler structure (i.e., a Banach norm on each tangent space of M, varying in a suitably regular way, inducing a complete distance on M).

A Nonlinear Elliptic Boundary-Value Problem

Let us consider a typical application of the mountain-pass theorem to a semilinear elliptic boundary-value problem. Let Ω be a smooth bounded domain in $\mathbb{R}^n$, and for $\lambda \in \mathbb{R}$, $p > 2$, consider the problem

$$\begin{aligned} -\Delta u &= \lambda u + u|u|^{p-2} && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \end{aligned} \qquad [1]$$

Let $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$ be the eigenvalues of the Laplace operator $-\Delta$, with domain $H^2 \cap H_0^1(\Omega)$, the Sobolev space of L^2-functions on Ω with weak first

two derivatives in L^2, vanishing on $\partial\Omega$. We claim that, if $n=2$, or if $n \geq 3$ and $2 < p < 2^* := 2n/(n-2)$, then problem [1] with $\lambda < \lambda_1$ has a nontrivial solution.

By elliptic regularity, the solutions of [1] are precisely the critical points of the functional

$$\mathcal{E}(u) = \frac{1}{2}\int_\Omega \left(|\nabla u(x)|^2 - \lambda u(x)^2\right) \mathrm{d}x - \frac{1}{p}\int_\Omega |u(x)|^p \, \mathrm{d}x$$

We recall that $H_0^1(\Omega)$ continuously embeds into $L^p(\Omega)$, for every $p < +\infty$ if $n=2$, for every $p \leq 2^*$ if $n \geq 3$. So the functional $\mathcal{E}$ is well defined, and actually continuously differentiable, on $H_0^1(\Omega)$, a Hilbert space with the inner product

$$\langle u, v\rangle_{H_0^1(\Omega)} = \int_\Omega \nabla u(x) \cdot \nabla v(x) \, \mathrm{d}x$$

Since $p > 2$, near zero the quadratic part of the functional $\mathcal{E}$ dominates over the part with the L^p-norm. By the Rayleigh characterization of the first eigenvalue of the Laplacian,

$$\lambda_1 = \min_{u \in H_0^1(\Omega)\setminus\{0\}} \frac{\int_\Omega |\nabla u(x)|^2 \, \mathrm{d}x}{\int_\Omega u(x)^2 \, \mathrm{d}x}$$

the assumption $\lambda < \lambda_1$ implies that the quadratic part of $\mathcal{E}$ is positive definite. So we can find a small $\rho > 0$ such that

$$a := \inf_{\|u\|_{H_0^1(\Omega)} = \rho} \mathcal{E}(u) > 0$$

On the other hand, the fact that $p > 2$ implies that

$$\lim_{\mu \to +\infty} \mathcal{E}(\mu u) = -\infty$$

for every $u \neq 0$. Therefore, the sublevel $\{\mathcal{E} < a\}$ is not connected, and if we can prove the Palais–Smale condition, the mountain-pass theorem will imply the existence of a critical point u with $\mathcal{E}(u) \geq a > 0$, i.e., a nontrivial solution of [1].

In order to prove the Palais–Smale condition, notice that the expression for the differential of $\mathcal{E}$,

$$D\mathcal{E}(u)[v] = \int_\Omega \nabla u(x) \cdot \nabla v(x) \, \mathrm{d}x - \int_\Omega \left(\lambda u(x) + |u(x)|^{p-2} u(x)\right) v(x) \, \mathrm{d}x$$

and the compactness of the embedding of $H_0^1(\Omega)$ into $L^p(\Omega)$ for $p < 2^*$ imply that the gradient of $\mathcal{E}$ has the form

$$\nabla\mathcal{E}(u) = u + K(u) \qquad [2]$$

where $K : H_0^1(\Omega) \to H_0^1(\Omega)$ is a compact map, that is, it maps bounded sets into precompact ones. It is readily seen that when $\nabla\mathcal{E}$ has such a form, bounded Palais–Smale sequences are compact. Thus, it is enough to show that every Palais–Smale sequence is bounded. But this follows from the identity

$$p\mathcal{E}(u) - D\mathcal{E}(u)[u] = \left(\frac{p}{2} - 1\right) \int_\Omega \left(|\nabla u(x)|^2 - \lambda u(x)^2\right) \mathrm{d}x$$

together with the fact that the right-hand side term defines an equivalent norm on $H_0^1(\Omega)$, because $p > 2$ and $\lambda < \lambda_1$. This concludes the proof.

Actually, using the maximum principle one could show that under the same assumptions, problem [1] has a solution which is positive in Ω.

When $n \geq 3$ and $p = 2^* = 2n/(n-2)$, the functional f still exhibits a mountain-pass geometry, but the Palais–Smale condition fails. In fact, the embedding of $H_0^1(\Omega)$ into $L^{2^*}(\Omega)$ is not compact, so the map K appearing in [2] is not compact, and bounded Palais–Smale sequences need not have a converging subsequence. We recall that the noncompactness of the embedding of $H_0^1(\Omega)$ into $L^{2^*}(\Omega)$ is due to the fact that the quotient

$$S(u) = \frac{\int_\Omega |\nabla u(x)|^2 \, \mathrm{d}x}{\left(\int_\Omega |u(x)|^{2^*} \mathrm{d}x\right)^{2/2^*}}$$

is invariant under rescaling $u \mapsto u_\mu(x) = u(\mu x)$.

When $\lambda = 0$, the Pohožaev identity – an integral formula obtained by multiplying the equation by $x \cdot \nabla u(x)$ – can be used to prove that problem [1] has no nontrivial solutions, when Ω is a star-shaped domain other than the whole $\mathbb{R}^n$.

When $\lambda \neq 0$, the presence in the functional of an L^2-norm – which rescales differently – breaks the symmetry, and the existence of nontrivial solutions is again possible. Indeed, Brezis and Nirenberg have shown that problem [1] with $p = 2^*$ has a nontrivial solution provided that $n \geq 4$ and $0 < \lambda < \lambda_1$, or $n = 3$ and $\lambda^* < \lambda < \lambda_1$, for some $\lambda^* \in [0, \lambda_1]$ depending on the domain Ω.

The proof is based on the fact that there is a certain threshold $s > 0$, related to the best Sobolev constant obtained by taking the infimum of $S(u)$ over all $u \in H_0^1$ (the domain is irrelevant here), below which the Palais–Smale condition holds. That is, every sequence (u_h) such that $\mathcal{E}(u_h)$ converges to some b less than s, and $D\mathcal{E}(u_h)$ tends to zero, is compact. The proof of the mountain-pass theorem shows that the Palais–Smale condition is needed only at the minimax level c. In order to conclude, it is then enough to show that $c < s$. The value of c can be estimated by using the fact that the

infimum of the quotient S over functions on the whole $\mathbb{R}^n$ is attained at the family of functions

$$u^*(x) = \left(\frac{\epsilon^2 n(n-2)}{(\epsilon^2 + |x|^2)^2}\right)^{(n-2)/4}$$

which are then solutions of [1] with $p = 2^*, \lambda = 0$, and $\Omega = \mathbb{R}^n$.

Another way to break the symmetry is to keep $\lambda = 0$ but to consider domains with a rich topology. For instance, Bahri and Coron have shown that if Ω is a domain with some nonzero singular homology group $H_k(\Omega; \mathbb{Z}_2), k \geq 1$, then problem [1] with $p = 2^*$ and $\lambda = 0$ has a positive solution.

Elliptic equations having nonlinearities with the critical exponent 2^* arise naturally in some geometric problems. Consider a manifold M of dimension $n \geq 3$, with a metric g having scalar curvature k. The Yamabe problem calls for finding a metric g_0, conformally equivalent to g, having constant scalar curvature. If $g_0 = u^{4/(n-2)}g$, where the positive function u gives the conformal factor, one finds that u must solve the equation

$$-\frac{4(n-1)}{n-2}\Delta_g u = -ku + k_0 u|u|^{2^*-2}$$

where Δ_g is the Laplace–Beltrami operator associated with the metric g, and the constant k_0 is the scalar curvature of g_0. Again, the corresponding functional satisfies the Palais–Smale condition only below a certain threshold (actually, the same number s as seen earlier; this because the lack of compactness is due to local concentration phenomena, and the metric structure of the whole ambient becomes irrelevant). The task is then to show that the minimax level is below that threshold or, equivalently, that a certain best Sobolev constant for (M, g) is less than the corresponding constant for $\mathbb{R}^n$ with the flat metric (the latter constant is again the infimum of $S(u)$). This fact was proved by Aubin in the case $n \geq 6$ or (M, g) not locally conformally flat. Schoen has then treated the remaining case, by means of the positive-mass theorem, a deep result in differential geometry.

A General Minimax Principle

Let us consider again a twice continuously differentiable function f on a real Hilbert space H. The vector field

$$V(u) = \frac{\nabla f(u)}{\sqrt{1 + \|\nabla f(u)\|^2}}$$

has the same nice properties of the gradient vector field of f, but in addition it is bounded. The advantage is that the flow of $-V$ is globally defined. When talking about the negative-gradient flow of f, we will actually refer to such a flow. It will also be useful to dispose of a negative-gradient flow truncated below level b. This is the flow of the vector field $-V_b$, where

$$V_b(u) = \varphi(f(u))V(u)$$

with φ a smooth function on $\mathbb{R}$ which is identically zero on $[-\infty, b]$, then increases up to reaching the value 1, and afterwards remains constantly equal to 1. This truncated negative-gradient flow keeps the points in the sublevel $\{f \leq b\}$ fixed, and behaves as the negative-gradient flow above b (except the fact that trajectories slow down as the value of f approaches b).

After these preliminaries, let us consider again the characterization of the critical level c appearing in the mountain-pass theorem. This critical level was obtained as the infimum over a certain class Γ of sets γ – the curves with end points in different components of $\{f < a\}$ – of the maximum of f over γ. But if we look back at the proof, we realize that the fact that these sets were curves was not essential. The important feature was that the negative-gradient flow $\phi(t, \cdot)$ mapped a set of the class Γ into a set still belonging to the class Γ, for $t \geq 0$. This observation leads to the following general minimax theorem, due to Palais:

Theorem (General minimax). *Let f be a twice continuously differentiable function on a real Hilbert space H, satisfying the Palais–Smale condition. Let Γ be a class of subsets of H which is positively invariant under the action of the negative-gradient flow ϕ of f (possibly truncated below level b): that is, if the set γ belongs to Γ, then the set $\phi(t, \gamma)$ belongs to Γ for all $t \geq 0$. Then, if the number*

$$c := \inf_{\gamma \in \Gamma} \sup_{u \in \gamma} f(u)$$

is finite (and larger than b), then c is a critical value of f.

The proof goes along the same lines of the proof of the mountain-pass theorem: if c is not a critical value of f, the (possibly truncated) negative-gradient flow $\phi(t_0, \cdot)$ pulls a sublevel $\{f \leq c + \epsilon\}$ down into the sublevel $\{f \leq c - \epsilon\}$ (with $c - \epsilon > b$), for some large t_0, by the Palais–Smale condition. Then we achieve a contradiction choosing a set $\gamma \in \Gamma$ on which f does not exceed $c + \epsilon$, and noticing that $\phi(t_0, \gamma)$ is a set which still belongs to the class Γ, by positive invariance, and on which f does not exceed $c - \epsilon$.

As we shall see in the last section, the possibility of working with a truncated negative-gradient flow

(assuming in this case that $c > b$) makes the application of this theorem easier. Again, an analogous result holds for continuously differentiable functions on Banach spaces, or more generally on Banach manifolds with a complete Finsler structure.

Trivial classes Γ are the class of all points in H, and the class consisting of the single set H, yielding to the infimum and the supremum of f, respectively. More interesting classes are constructed by fixing a topological space X and considering the images of all continuous maps $h : X \to H$ belonging to a certain relative homotopy class.

Closed Geodesics on Compact Manifolds

A typical application of the general minimax theorem is Birkhoff proof of the existence of a closed geodesic on the sphere S^2, endowed with an arbitrary metric g. Closed geodesics are precisely the critical points of the energy functional

$$\mathcal{S}(x) = \frac{1}{2}\int_0^1 g(\dot{x}(t), \dot{x}(t))\, dt$$

on the Hilbert manifold $H^1(\mathbb{T}, S^2)$ consisting of all one-periodic loops on S^2 of Sobolev regularity H^1 (here $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ denotes the circle parametrized by $[0, 1]$). This functional satisfies the Palais–Smale condition and it is bounded below, but its minima are just the trivial constant loops, on which $\mathcal{S} = 0$.

Let us use angle coordinates (θ, φ) on S^2, $-\pi/2 \le \theta \le \pi/2, 0 \le \varphi \le 2\pi$ (θ is the latitude, φ the longitude). A (suitably regular) map $h : S^2 \to S^2$ induces a curve in $H^1(\mathbb{T}, S^2)$ parametrized by θ: the value of this curve at $\theta \in [-\pi/2, \pi/2]$ is the loop $t \mapsto h(\theta, 2\pi t)$. It is a curve that joins two constant loops. Let Γ be the set of curves in $H^1(\mathbb{T}, S^2)$ which are obtained by maps $h : S^2 \to S^2$ of topological degree 1. This class is clearly positively invariant under the action of the negative-gradient flow of $\mathcal{S}$ (as of every homotopy fixing the constant loops).

If we can show that the minimax level

$$c := \inf_{\gamma \in \Gamma} \sup_{u \in \gamma} \mathcal{S}(x)$$

is positive, we will get a positive critical value of $\mathcal{S}$ by the general minimax theorem, hence a nontrivial closed geodesic. By considering the fact that loops with small energy also have a small diameter, it is easy to construct a homotopy on $\{\mathcal{S} < a\}$, for some small $a > 0$, which shrinks every loop to a point. If $h : S^2 \to S^2$ determines a curve γ with $\max_{x \in \gamma} \mathcal{S}(x) < a$, composition with this homotopy yields to a homotopy of h to a map whose image is a curve in S^2. A further homotopy then shows that the map h is homotopic to a constant, which is impossible if h has degree 1. This shows that $c \ge a > 0$, concluding the proof.

Actually, Ljusternik and Fet have proved that every compact manifold M has a nontrivial closed geodesic. Indeed, if M has nonzero fundamental group, it is enough to minimize $\mathcal{S}$ on some nontrivial homotopy class of loops. Otherwise, the fact that M is a compact manifold implies that some homotopy group $\pi_{k+1}(M), 1 \le k < \dim M$, does not vanish. A construction similar to the one described above then allows to associate with every noncontractible map $h : S^{k+1} \to M$ a map $u : (B^k, \partial B^k) \to (H^1(\mathbb{T}, M), \{\mathcal{S} = 0\})$ which is not homotopically trivial (here B^k denotes the closed unit ball in $\mathbb{R}^k$, and the notation means that u maps the boundary of the ball B^k into the set of constant loops). Taking a minimax over the set of images of the maps u associated with every noncontractible map $h : S^{k+1} \to M$ yields to the desired critical point of $\mathcal{S}$ with positive energy.

It is conjectured that every compact manifold has infinitely many closed geodesics. Morse theory allows to prove this fact for the vast majority of manifolds, but not for the spheres. Bangert and Franks have established the existence of infinitely many geodesics on S^2 by proving that every area-preserving homeomorphism of the open disk with two fixed points must have infinitely many periodic points. Proving the existence of infinitely many closed geodesics on higher-dimensional spheres is a challenging open problem.

A Rigidity Property of a Certain Class of Maps

It is important that the class Γ in the general minimax theorem is only required to be invariant under the action of the negative-gradient flow, and not, say, under the action of any continuous homotopy on which the function f is nonincreasing. Indeed, too many undesirable things can be done on an infinite-dimensional Hilbert space by arbitrary continuous maps, whereas the maps arising from our negative-gradient flow might show some rigidity, forcing them to behave as maps on finite-dimensional spaces.

Let us clarify this point by considering the following example, due to Benci and Rabinowitz. It may sound a bit artificial at this moment (simpler examples could be built), but we will find it useful in the next section. Assume that our Hilbert space is

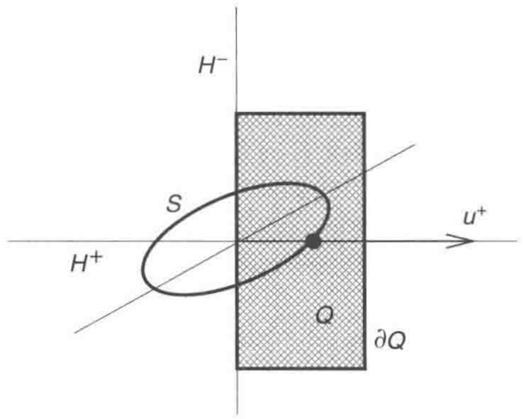


Figure 1 The sets $S, Q, \partial Q$.

endowed with an orthogonal splitting $H = H^- \oplus H^+$, fix a unit vector u^+ in H^+, and consider the sets

$$S = \{u \in H^+ \mid \|u\| = \rho\}$$
$$Q = \{u + \lambda u^+ \mid u \in H^-, \ \|u\| \leq \sigma, \ 0 \leq \lambda \leq \tau\}$$
$$\partial Q = \{u + \lambda u^+ \in Q \mid \lambda \in \{0, \tau\} \text{ or } \|u\| = \sigma\}$$

for some positive numbers ρ, σ, τ such that $\tau > \rho$. The latter inequality implies that the intersection $Q \cap S$ is not empty (see **Figure 1**).

If the linear subspace H^- is finite dimensional, a simple argument involving the topological degree shows the following fact: the image of any continuous map $h: Q \to H$ which is the identity on ∂Q has nonempty intersection with S.

When H^- is infinite dimensional, this fact is not true anymore. Indeed, it is not difficult to see that the set Q is homeomorphic to an infinite-dimensional closed ball B, by a homeomorphism ψ mapping ∂Q onto the infinite-dimensional sphere ∂B. If B is the closed ball of an infinite-dimensional Hilbert space, for instance, the space ℓ_2 of all square-summable sequences (x_h) endowed with the norm $|x|_2 = (\sum_{h=0}^{\infty} |x_h|^2)^{1/2}$, the continuous map

$$g(x_0, x_1, x_2, \ldots) = \left(\sqrt{1 - |x|_2^2}, x_0, x_1, x_2, \ldots\right)$$

maps B into ∂B and is a shift operator on ∂B. In particular, it is a continuous map on B without fixed points, and it can be used to define a map $h: B \to \partial B$ which is the identity on ∂B, by setting

$$h(x) = \mu(x)x + (1 - \mu(x))g(x)$$
$$\text{with } \mu(x) \geq 1 \text{ such that } |h(x)|_2 = 1$$

Conjugation by the homeomorphism ψ produces a continuous map from Q to ∂Q, which is the identity on ∂Q, providing us with the desired counterexample.

In other terms, when H^- is infinite dimensional, the sets ∂Q and S can be unlinked by means of a continuous map. The situation changes if we restrict the class of maps $h: Q \to H$ to those of the form

$$h(u) = u + K(u) \qquad [3]$$

where K is a continuous compact map. In this case, indeed, the argument for a finite-dimensional H^- can be applied, by replacing the topological degree by the Leray–Schauder degree (which is invariant precisely with respect to homotopies of the form above), and one proves that ∂Q and S cannot be unlinked by means of continuous maps of this form.

Closed Characteristics on Compact Energy Hypersurfaces

Consider $\mathbb{R}^{2n}$ with coordinates $(p_1, \ldots, p_n, q_1, \ldots, q_n)$, endowed with the standard symplectic form

$$\omega := \mathrm{d}p \wedge \mathrm{d}q = \sum_{j=1}^{n} \mathrm{d}p_j \wedge \mathrm{d}q_j$$

Let Σ be a compact connected hypersurface in $\mathbb{R}^{2n}$. The restriction of ω to the tangent space $T_x\Sigma$ has a one-dimensional kernel, which varies smoothly with x. In other words, there is a smooth line bundle

$$\mathcal{L}_\Sigma := \{(x, u) \in T\Sigma \mid \omega(u, v) = 0 \ \forall v \in T_x\Sigma\}$$

over Σ. We wish to discuss the classical problem of finding a closed characteristic for $\mathcal{L}_\Sigma$, that is, a closed curve everywhere tangent to $\mathcal{L}_\Sigma$.

This geometric problem has a dynamical interpretation. Indeed, let H be a smooth real function on $\mathbb{R}^{2n}$ such that Σ is the inverse image of the regular value 1. The function H – the Hamiltonian – generates a vector field X_H on $\mathbb{R}^{2n}$ by the formula

$$\omega(X_H(x), u) = -DH(x)[u], \quad \forall u \in \mathbb{R}^{2n}$$

or, equivalently,

$$X_H(x) = J\nabla H(x), \quad \text{with } J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$$

The Hamiltonian vector field X_H is tangent to Σ and belongs to $\mathcal{L}_\Sigma$. Therefore, the hypersurface Σ is invariant for the flow of X_H, and the flow orbits are precisely the characteristics. So finding a closed characteristic on Σ is equivalent to finding a periodic orbit of X_H with energy $H = 1$.

Up to changing the Hamiltonian, we may assume that all the values in an interval $]1 - \delta_0, 1 + \delta_0[$ are regular for H, and that the corresponding level sets $\Sigma_\eta := \{H = \eta\}$ are all connected (hence diffeomorphic to $\Sigma = \Sigma_1$). We would like to sketch Hofer and Zehnder's proof of the fact that there is a dense set of values $\eta \in]1 - \delta_0, 1 + \delta_0[$ for which Σ_η admits a closed characteristic.

This proof is based on the fact that the one-periodic orbits of X_H are critical points of the action functional

$$\mathcal{A}_H(x) = \int_{\mathbb{T}} x^*(p\,\mathrm{d}q - H\,\mathrm{d}t) = \frac{1}{2}\int_0^1 \dot{x}(t)\cdot Jx(t)\,\mathrm{d}t - \int_0^1 H(x(t))\,\mathrm{d}t$$

on the space of loops $x : \mathbb{T} \to \mathbb{R}^{2n}$.

Clearly, it is enough to show that for every $\delta > 0$ there is a closed characteristic on some Σ_η with $|\eta - 1| < \delta$. We can take advantage of the fact that we are free to change the Hamiltonian, as long as it has the level sets $\Sigma_\eta, |\eta - 1| < \delta$. Denoting by B the bounded component of the complement of $\{1-\delta \le H \le 1+\delta\}$, we may assume that B contains the origin. We can modify H in such a way that H vanishes identically on B, then it grows, parametrizing all the hypersurfaces $\Sigma_\eta, |\eta - 1| < \delta$, in a strictly increasing way, then it remains constant in a large ball, and finally it smoothly switches to the quadratic form $(3/2)\pi|x|^2$. By choosing H in this way, one can ensure that all the constant orbits and all the one-periodic orbits which do not lie on Σ_η for some $|\eta - 1| < \delta$ have non-positive action. So it is enough to prove that the functional $\mathcal{A}_H$ has a positive critical value.

Using the Fourier series decomposition

$$x(t) = \sum_{k\in\mathbb{Z}} \mathrm{e}^{2\pi ktJ}\hat{x}_k, \quad \hat{x}_k \in \mathbb{R}^{2n}$$

one sees that the quadratic part of the action functional has the form

$$\int_0^1 \dot{x}(t)\cdot Jx(t)\,\mathrm{d}t = 2\pi\sum_{k\in\mathbb{Z}} k|\hat{x}_k|^2 \qquad [4]$$

so it is positive on an infinite-dimensional linear space, negative on an infinite-dimensional linear space, and null on the $2n$-dimensional space spanned by the constant loops. The specific form of [4] suggests to choose as domain of the action functional the Sobolev space $H^{1/2}(\mathbb{T}, \mathbb{R}^{2n})$, the space of square-integrable one-periodic curves x in $\mathbb{R}^{2n}$ with

$$\|x\|^2_{H^{1/2}} := |\hat{x}_0|^2 + 2\pi\sum_{k\in\mathbb{Z}} |k||\hat{x}_k|^2 < +\infty$$

This is indeed a Hilbert norm on $H^{1/2}(\mathbb{T}, \mathbb{R}^{2n})$. The functional $\mathcal{A}_H$ is smooth on this space, and its gradient takes the form

$$\nabla\mathcal{A}_H(x) = Lx + K(x) \qquad [5]$$

where L is the self-adjoint Fredholm operator representing the quadratic form [4] with respect to the $H^{1/2}$-Hilbert product, and K is a compact map. A gradient of the form [5] again implies that bounded Palais–Smale sequences are compact. The Palais–Smale condition then follows from the fact that the Hamiltonian H is quadratic outside a large ball, and has no one-periodic orbits there (the large orbits are all periodic, but their period is 2/3).

Consider the splitting $H^{1/2}(\mathbb{T}, \mathbb{R}^{2n}) = H^- \oplus H^+$, with

$$H^- = \{x \mid \hat{x}_k = 0 \text{ for } k > 0\}$$
$$H^+ = \{x \mid \hat{x}_k = 0 \text{ for } k \le 0\}$$

Let S, Q, and ∂Q be the sets defined in the previous section, with

$$u^+(t) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{2\pi tJ}u_0, \quad u_0 \in \mathbb{R}^{2n},\ |u_0| = 1$$

and constants ρ, σ, τ to be determined. Since the quadratic form [4] is positive on H^+ and the Hamiltonian H vanishes near the origin, we can find a small $\rho > 0$ such that

$$\inf_{x\in S} \mathcal{A}_H(x) > 0$$

The fact that the quadratic form [4] is seminegative on H^- and the behavior of $H(x)$ for large $|x|$ imply that if σ and τ are suitably large (in particular $\tau > \rho$), then

$$\sup_{x\in\partial Q} \mathcal{A}_H(x) \le 0$$

Let Γ be the set of all images of maps

$$h : Q \to H^{1/2}(\mathbb{T}, \mathbb{R}^{2n})$$

which are the identity on ∂Q and are of the form

$$h(x) = \mathrm{e}^{\alpha(x)L}(x + K(x)) \qquad [6]$$

with α a continuous real-valued function, and K a continuous compact map. This class of maps is more general than the one considered in the previous section, but the fact that $\mathrm{e}^{\alpha L}$ commutes with the projections onto H^- and H^+ ensures that ∂Q and S cannot be unlinked even inside this class. Therefore, any $\gamma \in \Gamma$ has nonempty intersection with S, so

$$c := \inf_{\gamma\in\Gamma}\sup_{x\in\gamma} \mathcal{A}_H(x) \ge \inf_{x\in S}\mathcal{A}_H(x) > 0$$

We would like to apply the general minimax theorem, and conclude that c is the desired positive critical value.

The number c being clearly finite, it is enough to show that Γ is positively invariant under the action of the negative-gradient flow ϕ of $\mathcal{A}_H$, truncated below level 0. Let $\gamma = h(Q) \in \Gamma$ and $t \ge 0$. Then $\phi(t, \gamma)$ is the image of Q by the map $\phi(t, h(\cdot))$. This

map is the identity on ∂Q because ∂Q lies in $\{\mathcal{A}_H \leq 0\}$ and ϕ is truncated below level 0. It is of the form [6] because by [5] the truncated negative-gradient flow of $\mathcal{A}_H$ has the form

$$\phi(t,x) = e^{-\theta(t,x)L}(x + K(t,x))$$

for some continuous function $0 \leq \theta(t,x) \leq t$ and for some continuous compact map K. This concludes the proof.

This result was refined by Struwe, who proved the existence of a closed characteristic on Σ_η for almost every η, in the sense of the Lebesgue measure. We could try to use the abundance of closed characteristics on energy levels near Σ to get the existence of one on Σ by taking a limit. But this process produces a closed characteristic on Σ only if we can bound the periods of the approximating closed orbits, otherwise a more general invariant set results. Actually, Ginzburg, Herman, and Gürel have produced examples of compact hypersurfaces without any closed characteristic.

As conjectured by Weinstein and proved by Viterbo, closed characteristics always exist on contact-type compact hypersurfaces (i.e., hypersurfaces Σ on which the restriction of ω is the differential of a 1-form λ such that $\lambda \wedge d\lambda \wedge \cdots \wedge d\lambda$ is a volume form). In this case, one should even expect a multiplicity result. For hypersurfaces which bound a strictly convex set in $\mathbb{R}^{2n}$, for instance, the existence of n closed characteristics is conjectured. The best result so far is due to Long, who could prove the existence of $[n/2]+1$ of them. Hofer, Wysocki, and Zehnder have proved that, when $n=2$, there are either two or infinitely many closed characteristics (for a generic contact-type hypersurface diffeomorphic to S^3), by using the already mentioned theorem by Franks on periodic points of area-preserving homeomorphisms of the disk. Proving an analogous result for $n \geq 3$ is an intriguing open problem.

See also: Contact Manifolds; Floer Homology; Hamilton–Jacobi Equations and Dynamical Systems: Variational Aspects; Image Processing: Mathematics; Inequalities in Sobolev Spaces; Leray–Schauder Theory and Mapping Degree; Ljusternik–Schnirelman Theory; Saddle Point Problems.

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Mirror Symmetry: A Geometric Survey

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Introduction

Mirror symmetry was discovered in the late 1980s by physicists studying superconformal field theories (SCFTs). One way to produce SCFTs is from closed string theory; in the Riemannian (rather than Lorentzian) theory the string's world line gives a map of a Riemannian 2-manifold into the target with an action which is conformally invariant, so the 2-manifold can be thought of as a Riemann surface with a complex structure. Making sense of the infinities in the quantum theory (supersymmetry and anomaly cancelation) forces the target to be 10-dimensional – Minkowski space times by a 6-manifold X – and X to be (to first order) Ricci flat and so to have holonomy in SU(3). That is X is a Calabi–Yau 3-fold (X, Ω, ω). So SCFTs come from σ-models (mapping Riemann surfaces into Calabi–Yau 3-folds) but, it turns out, in two different ways – the A-model and the B-model. Deformations of the SCFT and either σ-model are isomorphic, so over an open set the two coincide. Thus, it was natural to conjecture that almost all of the relevant SCFTs came from geometry – from an A or B σ-model. In particular,

the A-model of a Calabi–Yau X should, therefore, give the same SCFT as the B-model on another Calabi–Yau $\check{X}$. It turns out then that the A-model on $\check{X}$ should also be isomorphic to the B-model on X; thus, mirror symmetry should give an involution on a Calabi–Yau 3-folds. (The full picture is slightly more complicated – it involves large complex structure limits, multiple mirrors and flops.) By studying the SCFTs, Greene and Plesser predicted the mirror of the simplest Calabi–Yau 3-fold, the quintic in $\mathbb{P}^4$, and mirror symmetry was born.

Topological observables, that is, certain path integrals over the space of all maps, can be calculated by the semiclassical approximation as integrals over the space of classical minima – (anti) holomorphic curves in the Calabi–Yau (these minimize volume in a fixed homology class). From the zero homology class we get the constant maps – points in X – and so integrals over X. In some cases, by Poincaré duality, these can be thought of as intersections of cycles; we think of the string world sheet lying at a point of intersection. When the world sheet has a nontrivial homology class, it allows more general "intersections" where the cycles need not intersect but are connected by a holomorphic curve, giving a perturbation of the usual intersection product on cohomology called quantum cohomology. Namely, there is a contribution $(a.\beta)(b.\beta)(c.\beta)e^{\int_\beta \omega}$ to the quantum triple product $a.b.c$ of three 4-cycles $a, b, c \in H^{1,1} \cong H^2 \cong H_4$ from each holomorphic curve β (of genus 0, in the 0-loop approximation to the physics) in X of area $\int_\beta \omega$ (where ω is the Kähler form). The A-model correlation functions can be determined from these data; the B-model computation involves no such quantum correction and can be computed purely in terms of integrals over cycles ("periods") and their derivatives (discussed in the next section). So it is in some sense easier and, in a historic tour-de-force, was calculated by Candelas *et al.* (1991) for the Greene–Plesser mirror of the quintic. Comparing with the A-model computation on the quintic gave remarkable predictions about the number of holomorphic rational curves on the quintic. These were way beyond mathematical capabilities at the time, and sparked enormous mathematical interest. The predictions (and more) have now been proved to be true by Givental and Lian–Liu–Yau, while mirror symmetry has begun to be understood geometrically. But, in some sense, the mathematical reason for the relationship between the Yukawa couplings and the quantum cohomology of the mirror is still a little mysterious; it is the hardest part of mirror symmetry to see in the geometry, yet for the physics it was the easiest and the first prediction.

We survey, nonchronologically, some of the geometry of mirror symmetry as it is now understood, mainly in dimension $n=3$. For the many topics omitted, the reader should consult the Further Reading section.

The Geometric Setup

A Calabi-Yau 3-fold (X, Ω, ω) is a Kähler manifold (X, ω) with a holomorphic trivialization Ω of its canonical bundle

$$K_X = \Lambda^3_{\mathbb{C}} T^* X$$

(i.e., a nowhere-vanishing holomorphic volume form, locally $dz_1 \wedge dz_2 \wedge dz_3$), and $b_1(X) = 0$. It follows that the Hodge numbers $h^{0,2}, h^{0,1}$ vanish, and so $H^2(X, \mathbb{C}) = H^{1,1}$ and $H^3(X, \mathbb{R}) \cong H^{2,1} + H^{3,0}$. By Yau's theorem the Kähler metric can be changed within its $H^2(X, \mathbb{R})$ cohomology class to a unique Ricci-flat Kähler metric; equivalently, Ω is parallel, so the induced metric on K_X is flat. Roughly speaking, mirror symmetry swaps the symplectic or Kähler structure ω on X with the complex structure (encoded in Ω, up to scaling by $\mathbb{C}^*$) on the (conjectural) mirror $\check{X}$. Kähler deformations are unobstructed, forming an open set $\mathcal{K}_X$ in $H^2(X, \mathbb{R})$. Its closure $\overline{\mathcal{K}}_X$ is sometimes extended by adding the Kähler cones of all birational models of X to give Kawamata's movable cone. This is because the work of Aspinwall, Greene, Morrison, and Witten suggested that all birational models of X are indistinguishable in string theory and so are all mirrors of $\check{X}$, corresponding to a different choice of $(1,1)$-form ω which is a Kähler form on one model only. $\mathcal{K}_X$ is also complexified by including in the A-model data any "B-field" $B \in H^2(X, \mathbb{R}/\mathbb{Z})$, and divided by holomorphic automorphisms of X, to give a moduli space of complex dimension $h^{1,1}(X)$. Deformations of complex structure are also unobstructed by the nontrivial Bogomolov–Tian–Todorov theorem; thus, they form a smooth space with tangent space

$$H^1(T\check{X}) \xrightarrow[\simeq]{\lrcorner \Omega} H^1(\Lambda^2 T^* \check{X}) = H^{2,1}(\check{X})$$

(Given a deformation of complex structure, the above isomorphism takes the $H^{2,1}$-component of the derivative of the $(3,0)$-form Ω.) So, for the moduli spaces to match up, we get the first and simplest prediction of mirror symmetry:

$$h^{1,1}(X) = h^{2,1}(\check{X}) \quad \text{and} \quad h^{2,1}(X) = h^{1,1}(\check{X}) \qquad [1]$$

This is where mirror symmetry gets its name, the above relation making the Hodge diamonds of X and $\check{X}$ mirror images of each other.

As the complexified Kähler cone is a tube domain, it has natural partial complex compactifications (due to Looijenga, and suggested in the context of mirror symmetry by Morrison (1993)). The simplest case is where we ignore the movable cone and automorphisms and assume that there is an integral basis $e_1, \ldots, e_n$ of both $\overline{\mathcal{K}}_X$ and $H^2(X, \mathbb{Z})$/torsion. The complexified Kahler moduli space is then

$$\mathcal{K}_X^{\mathbb{C}} := H^2(X, \mathbb{R})/H^2(X, \mathbb{Z}) + \mathrm{i}\mathcal{K}_X = \{B + \mathrm{i}\omega\}$$

with natural coordinates $x_i, y_i \geq 0$ pulled back from the first and second factors, respectively, induced by the e_i. x_i is multivalued with integer periods, so

$$z_i = \exp(2\pi \mathrm{i}(x_i + \mathrm{i}y_i)) \qquad [2]$$

is a well-defined holomorphic coordinate, giving an isomorphism to the product of n punctured unit disks in $\mathbb{C}$:

$$\mathcal{K}_X^{\mathbb{C}} \cong (\Delta^*)^n = \{(z_i) : 0 < |z_i| \leq 1\} \subset (\mathbb{C}^*)^n$$

The compactification Δ^n comes from adding in the origins in the disks, which we reach by going to infinity (in various directions) in $\mathcal{K}_X^{\mathbb{C}}$. We call the point $(0, \ldots, 0) \in \Delta^n$ the large Kahler limit point (LKLP) in this case. Moving along the ray generated by $\sum k_i e_i \in \mathcal{K}_X, k_i \geq 0$, complexifies in the holomorphic structure [2] to give the analytic curve

$$z_i^{k_j} = z_j^{k_i}, \quad \forall i, j \qquad [3]$$

in $\mathcal{K}_X^{\mathbb{C}}$. For $k_i \in \mathbb{Q}\ \forall i$, this extends to a complete curve in the compactification. Without loss of generality, we can assume that k_i are integers with no common factor; then the link of the curve winds around the LKLP $(0, \ldots, 0) \in \Delta^n$ with winding number

$$\begin{aligned}(k_1, \ldots, k_n) &\in \pi_1(H^2(X, \mathbb{R})/H^2(X, \mathbb{Z}) + \mathrm{i}\mathcal{K}_X) \\ &= H^2(X, \mathbb{Z}) = \mathbb{Z}.e_1 \oplus \cdots \oplus \mathbb{Z}.e_n\end{aligned}$$

This is because multiplying the ray $\mathbb{R}.\Sigma k_i e_i \in \mathcal{K}_X$ by i gives the direction $\mathbb{R}.\Sigma k_i e_i$ in the space $H^2(X, \mathbb{R})/H^2(X, \mathbb{Z})$ of B-fields, with the given winding number. For k_i not rational we get an analytic mess; the direction in the space of B-fields does not close up to give a circle.

There is no obvious mirror to these rays since we consider Ω only up to scale. So, mirror symmetry predicts an isomorphism between $\mathcal{K}_X^{\mathbb{C}}$ and the moduli space $\mathcal{M}_{\check{X}}$ of complex structures on $\check{X}$, and a distinguished limit in $\mathcal{M}_{\check{X}}$, the large complex structure limit point (LCLP), the mirror of the LKLP $(0, \ldots, 0) \in \Delta^n$ above. Morrison has given a rigorous definition of LCLPs and the canonical coordinates on $\mathcal{M}_{\check{X}}$ dual to the z_i on $\mathcal{K}_X^{\mathbb{C}}$; see the section Monodromy around the LCLP. The holomorphic curves in $(\Delta)^n$ described above, corresponding to rational rays of Kähler forms, give degenerations of (the complex structure on) $\check{X}$ to the LCLP whose monodromy is discussed in this article (see "Lagrangian Torus Fibrations").

LCLPs play a vital role in mirror symmetry; in fact, mirror symmetry is really a statement about LCLPs and families of Calabi–Yau manifolds near LCLPs. Most predictions only really hold near or at the LCLP, and the complex structure moduli space only looks like Δ^n near the LCLP. For instance, manifolds can have many LCLPs and accordingly many mirrors. This also explains one obvious paradox – that rigid Calabi–Yau manifolds, those with no complex structure deformations, $h^{2,1} = 0$, and so no LCLP, can have no mirror, since a Kähler (or symplectic) manifold has $h^2 = h^{1,1} \neq 0$.

The first predicted refinement of [1] is, as discussed in the introduction, that the variation of Hodge structure (VHS) on $\check{X}$ should be describable in terms of Gromov–Witten invariants of X. Here VHS is governed by how the ray $\mathbb{C}.\Omega_t = H^{3,0}(\check{X}_t)$ sits inside $H^3(\check{X}_t, \mathbb{C})$ as the complex structure on $\check{X}_t$ varies, parametrized by $t \in \mathcal{M}_{\check{X}}$. By Poincaré duality, it is sufficient to know how Ω_t pairs with $H_3(\check{X})$, that is, to compute the period integrals

$$\int_{A_i} \Omega_t, \quad i = 1, \ldots, 2k = 2h^{2,1} + 2$$

where A_i form a basis of $H_3(\check{X}, \mathbb{Z})$. (In fact we can choose the A_i to be a symplectic basis, $A_i.A_j = \delta_{i+k,j}$, and then knowledge of only the periods of the first k A_i suffices, locally in moduli space.) These periods determine Ω_t and so the Yukawa coupling

$$H^1(T\check{X}_t)^{\otimes 3} \xrightarrow{\cup} H^3(\Lambda^3 T\check{X}_t) \xrightarrow{\lrcorner \Omega_t^{\otimes 2}} H^3(K_{\check{X}_t}) \cong \mathbb{C} \qquad [4]$$

On X, we get the cubic form on $H^2(X)$ described earlier in terms of numbers of rational curves in X. These numbers are in fact independent of the almost-complex structure on X (as long as it is compatible with the symplectic form ω), and, therefore, give the symplectic invariants of Gromov and Witten. The cubic form depends on $\omega = \omega_t$ as it moves in $\mathcal{K}_{X_t}$ (or in $\mathcal{K}_{X_t}^{\mathbb{C}}$, replacing ω_t by $-\mathrm{i}(B_t + \mathrm{i}\omega_t)$). Under the predicted local isomorphism $\mathcal{K}_X^{\mathbb{C}} \cong \mathcal{M}_{\check{X}}$ near the LKLP and LCLP, the equality of these cubic forms gives the predictions of number of rational curves in X mentioned in the introduction. This has been carried out, and the predictions checked rigorously, in quite some generality, for instance for mirror pairs produced by Batyrev's toric methods.

There is, of course, a flat connection, the Gauss–Manin connection on the bundle over $\mathcal{M}_{\check{X}}$ with fiber $H^3(\check{X}_t, \mathbb{C})$ over $t \in \mathcal{M}_{\check{X}}$, given by the local system $H^3(\check{X}_t, \mathbb{Z}) \subset H^3(\check{X}_t, \mathbb{C})$. As mirror to this, Dubrovin has shown how to put a flat connection on the bundles with fibers $H^2(X_t)$ and $H^{\mathrm{ev}}(X_t)$ using Gromov–Witten invariants.

Homological Mirror Symmetry

Building on the work of Witten, Kontsevich (1995) proposed a remarkable conjecture that purported to explain mirror symmetry, all the more surprising because it appeared to have little to do with what was thought to be mirror symmetry at the time. The conjecture is now reasonably well understood, while the link to Gromov–Witten invariants and Yukawa couplings is more mysterious, although it is known how both data should be encoded in the conjecture.

Kontsevich proposed that mirror symmetry should be explained by a (noncanonical) equivalence of triangulated categories between the derived Fukaya category $D^{\mathcal{F}}(X)$ of (X, ω) and the bounded derived category of coherent sheaves $D^{\mathrm{b}}(\check{X})$ on its mirror $\check{X}$. This second category consists of chain complexes of holomorphic bundles, with quasi-isomorphisms (maps of chain complexes which induce isomorphisms on cohomology) formally inverted, that is, decreed to be isomorphisms. For zero B-field the first category should be constructed from Lagrangian submanifolds $L \subset X$ carrying flat unitary connections A. That is, L is middle- (three-) dimensional, and

$$\omega|_L \equiv 0, \qquad F_A = 0$$

For $B \neq 0$, this needs modifying to $F_A + 2\pi i B.\mathrm{id} = 0$ (so, in particular, we require that L satisfies $[B|_L] = 0 \in H^2(L, \mathbb{R}/\mathbb{Z})$). There are also various technical conditions such as the choice of a relative spin structure, the Maslov class of L must vanish (i.e., the map $(\Omega|_L/\mathrm{vol}_L) : L \to \mathbb{C}^*$ has winding number zero) and we pick a grading on L (a choice of logarithm of this map). Morphisms are defined by Floer cohomology HF^* of Lagrangian submanifolds; roughly speaking, this assigns a vector space to each intersection point (the homomorphisms between the fibers of the two unitary bundles carried by the Lagrangians at this point), made into a chain complex by a certain counting of holomorphic disks between intersection points. In-depth work by Fukaya–Oh–Ohta–Ono shows that this gives the structure of an A^∞-category which can then be "derived" into a triangulated category in a formal way by taking "twisted cochains." The construction is still very technical and difficult to calculate with, but the key points are that we get a category depending only on the symplectic structure, that certain "unobstructed" Lagrangian submanifolds give objects of this category, and that Hamiltonian isotopic unobstructed Lagrangian submanifolds give isomorphic objects.

Since the introduction of D-branes there is a physical interpretation of this conjecture in terms of open string theory; the objects of the two categories are boundary conditions for open strings, and morphisms correspond to strings beginning on one object and ending on the other. So, for instance, intersections of Lagrangians give morphisms corresponding to constant strings at the intersection point, while the Floer differential gives instanton tunneling corrections.

One paradox this formulation immediately sheds light on concerns automorphisms on both sides of mirror symmetry. While symplectomorphisms of (X, ω) are abundant, there are few holomorphic automorphisms of a Calabi–Yau $\check{X}$. The former induce autoequivalences of $D^{\mathcal{F}}(X)$; Kontsevich's suggestion is that as a mirror to this there should be an autoequivalence of $D^{\mathrm{b}}(\check{X})$; this need not be induced by an automorphism of $\check{X}$. Motivated by this, groups of autoequivalences of derived categories of sheaves of Calabi–Yau manifolds have now been found that were predicted by mirror symmetry; a few are mentioned below. Thus, homological mirror symmetry suggests that an SCFT is equivalent to a triangulated category, and the ambiguities in geometrizing an SCFT (finding a Calabi–Yau of which it is a σ-model) are seen in the category – not all automorphisms come from an automorphism of a Calabi–Yau (e.g., Calabi–Yau manifolds $\check{X}$ with equivalent derived categories give multiple mirrors to X), and not all appropriate categories need even come from a Calabi–Yau. Supporting this suggestion, Bondal–Orlov and Bridgeland have shown that indeed birational Calabi–Yau manifolds $\check{X}$ have equivalent derived categories.

Finally, Kontsevich explained how deformation theory of the categories should involve derived morphisms on the product from the diagonal (thought of as a Lagrangian in the A-model, its structure sheaf as a coherent sheaf in the B-model) to itself, giving quantum cohomology in the A-model and Hodge structure in the B-model. For instance, the holomorphic disks used to compute the Floer cohomology of the diagonal on the product $X \times X$ give holomorphic rational curves on X. So, one should be able to see some parts of "classical" mirror symmetry.

Below, as we describe more of the geometry of mirror symmetry that has emerged since Kontsevich's conjecture, we will mention at each stage how his conjecture fits in with it.

The Strominger–Yau–Zaslow Conjecture

To recover more geometry from Kontsevich's conjecture, there are some obvious objects of $D^b(\check{X})$ that reflect the geometry of $\check{X}$ – the structure sheaves $\mathcal{O}_p$ of points $p \in \check{X}$. Calculating their self-Homs, $\mathrm{Ext}^*(\mathcal{O}_p, \mathcal{O}_p) \cong \Lambda^* T_p\check{X} \cong \Lambda^*\mathbb{C}^3 \cong H^*(T^3, \mathbb{C})$, shows that if they are mirror to Lagrangians L in X (with flat connections A on them) then we must have

$$HF^*((L, A), (L, A)) \cong H^*(T^3, \mathbb{C})$$

as graded vector spaces. Since the left-hand side is, modulo instanton corrections, $H^*(L, \mathbb{C})^{\oplus r}$, where r is the rank of the bundle carried by L, this suggests that the mirror should be $L \cong T^3$ with a flat U(1) connection A over it. There are reasons why the Floer cohomology of such an object should not be quantum corrected, and so be isomorphic to $\mathrm{Ext}^*(\mathcal{O}_p, \mathcal{O}_p)$.

For any Lagrangian L, the symplectic form gives an isomorphism between T^*L and its normal bundle N_L; thus, Lagrangian tori have trivial normal bundles, and locally one can fiber X by them. Thus, one might hope that X is fibered by Lagrangian tori, and the mirror $\check{X}$ is (at least over the locus of smooth tori) the dual fibration. This is because the set of flat U(1) connections on a torus is naturally the dual torus.

This is the kind of philosophy that led to the Strominger–Yau–Zaslow (SYZ) conjecture (Strominger *et al.* 1996), although Strominger *et al.* were working with physical D-branes, and not Kontsevich's conjecture. Therefore, their D-branes are not the "topological D-branes" of Kontsevich, but those minimizing some action. That is, instead of holomorphic bundles in the B-model, we deal with bundles with a compatible connection satisfying an elliptic partial differential equation (PDE) (e.g., the Hermitian–Yang–Mills equations (HYM), or some perturbation thereof); instead of Lagrangian submanifolds up to Hamiltonian isotopy in the A-model, we consider special Lagrangians (sLags) (see eqn [5]). The SYZ conjecture is that a Calabi–Yau X should admit a sLag torus fibration, and that the mirror $\check{X}$ should admit a fibration which is dual, in some sense.

A sLag is a Lagrangian submanifold of a Calabi–Yau manifold X satisfying the further equation that the unit norm complex function (phase)

$$\frac{\Omega|_L}{\mathrm{vol}_L} = \mathrm{e}^{\mathrm{i}\theta} = \text{constant} \qquad [5]$$

(So, sLags have Maslov class zero, in particular.) This equation uses the complex structure on X as well as the symplectic structure, and the resulting Ricci-flat metric of Yau, to define a metric on L and so its Riemannian volume form vol_L. SLags are calibrated by $\mathrm{Re}(\mathrm{e}^{-\mathrm{i}\theta}\Omega)$ and so minimize volume in their homology class. This is similar to the HYM equations on the mirror $\check{X}$, which are defined on holomorphic bundles on the complex manifold $\check{X}$ via a Kähler form ω, and minimize the Yang–Mills action. The Donaldson–Uhlenbeck–Yau theorem states that for holomorphic bundles that are polystable (defined using $[\omega]$, this is true for the generic bundle), there is a unique compatible HYM connection. Thus, modulo stability, HYM connections are in one-to-one correspondence with holomorphic bundles. A similar correspondence is conjectured, and proved in some special cases, by Thomas and Yau, for (special) Lagrangians: that modulo issues of stability (which can be formulated precisely), sLags are in one-to-one correspondence with Lagrangian submanifolds up to Hamiltonian isotopy. That is, there should be a unique sLag in the Hamiltonian isotopy class of a Lagrangian if and only if it is stable. Currently, only the uniqueness part of this conjecture has been worked out, but, in principle at least, we do not lose much by considering only Lagrangian torus fibrations.

The SYZ conjecture is thought to hold only near the LCLPs and LKLPs of X and $\check{X}$; away from these, the sLag fibers may start to cross. According to Joyce, the discriminant locus of the fibration on X is expected to be a codimension one ribbon graph in a base S^3 near the limit points, while the discriminant locus of the dual fibration $\check{X}$ may be different – that is, the smooth parts of the fibration and its dual are compactified in different ways. In the limit of moving to the limit points, however, both discriminant loci shrink onto the same codimension-two graph. In this limit, the fibers shrink to zero size, so that X (with its Ricci-flat metric) tends, in the Gromov–Hausdorff sense, to its base S^3 (with a singular metric). This formal picture has been made precise in two dimensions, for $K3$-surfaces, by Gross and Wilson. The limiting picture suggests that if we are only interested in topological or Lagrangian torus fibrations then we might hope for codimension-two discriminant loci, and such fibrations might make sense well away from limit points. Gross and Ruan carry this out in examples such as the quintic and its mirror, and makes sense of dualizing the fibration by dualizing monodromy around the discriminant locus

and specifying a canonical compactification over the discriminant locus. This gives the correct topology for toric varieties and their mirrors, and flips the Hodge numbers [1], for instance. Approaching the LCLP in a different way (in the example of eqn [3] this corresponds to altering the rational numbers k_i) can give a different graph and different fibration on X; the dual fibration can then be a topologically different manifold, giving a different birational model of the mirror $\check{X}$.

We focus only on Lagrangian fibrations, as they are better behaved and understood. We can expect them to be C^∞ fibrations with codimension-two discriminant loci, for instance. Below we see how to put a complex structure on the smooth part of the fibration, but extending this over the compactification is much harder and will involve "instanton corrections" coming from holomorphic disks. Fukaya (2005) has beautiful conjectures about this that will explain a great deal more of mirror symmetry, but they will not be discussed here.

Lagrangian Torus Fibrations

If $(X^{2n}, \omega) \xrightarrow{\pi} B^n$ is a *smooth* Lagrangian fibration with compact fibers, then the fibration is naturally an affine bundle of torus groups (i.e., a bundle of groups once we pick a Lagrangian 0-section – an identity in each fiber), and the base B inherits a natural integral affine structure: it looks like a vector space V with an integral structure $V \cong \Lambda \otimes_{\mathbb{Z}} \mathbb{R}$ up to translation by elements of V. This is the classical theory of action-angle variables. T_b^*B acts on the fiber $X_b = \pi^{-1}(b)$: by pullback and contraction with the symplectic form, $\sigma \in T_b^*B$ gives a vector field $\underline{\sigma}$ tangent to X_b, and the time-one flow along $\underline{\sigma}$ gives the action. By compactness and smoothness of X_b the kernel is a full-rank lattice $\Lambda_b \subset T_b^*B$, giving the isomorphism

$$X_b \cong T_b^*B/\Lambda_b$$

We define the integral affine structure on B by specifying the integral affine functions f (up to translation) to be those whose time-one flow along $\underline{df}$ is the identity (i.e., on the universal cover the time-one flow is to a section of the bundle of lattices Λ).

The situation that concerns us is where B is a 3-manifold $\bar{B}$ (usually S^3) minus a graph; then the monodromy around the graph preserves the integral affine structure:

$$\pi_1(B) \to \mathbb{R}^3 \rtimes GL(3, \mathbb{Z}) \qquad [6]$$

A great deal of mirror symmetry can be seen from just this knowledge of the smooth locus of the fibration; in particular, Gross (1998) has shown how mild assumptions about the compactification (with singular fibers over $\bar{B}\backslash B$) are enough to determine much of the topology of X. The dual fibration $\check{\pi}$ should have the monodromy dual to [6], and he shows how this implies the switching of the Hodge numbers [1] by the Leray spectral sequence; the rough idea being the obvious isomorphism

$$R^i\pi_*\mathbb{R} \cong \Lambda^i TB \cong \Lambda^{3-i}T^*B \cong R^{3-i}\check{\pi}_*\mathbb{R}$$

induced by a trivialization of $\Lambda^3 TB$. That is, morally speaking, the flipping of Betti numbers arises by representing cycles by those with linear intersection with the fibers, and replacing this linear space by its annihilator in the dual torus. This also agrees with the equivalence taking Lagrangians to coherent sheaves described in the next section.

The dual fibration $\check{\pi}$ has a natural complex structure; here the affine structure is essential, as in general a tangent bundle TB only has a natural almost complex structure along its 0-section. Since, up to translation, locally $B \cong V$ is a vector space, $TB \cong V \times V \cong V \otimes_{\mathbb{R}} \mathbb{C}$ has a natural complex structure which descends to

$$\check{\pi} : \check{X} = TB/\Lambda^* \to B \qquad [7]$$

Gross suggests that the B-field on X should lie in the piece

$$H^1(R^1\pi_*\mathbb{R}/\mathbb{Z}) = H^1(TB/\Lambda^*)$$

of the Leray spectral sequence converging to $H^2(X, \mathbb{R}/\mathbb{Z})$. That is, it is represented by a Čech cocycle e on overlaps of an open cover of B with values in the dual bundle of groups TB/Λ^*. Using this to twist [7] and re-glue it via transition functions translated by e, we get a new complex manifold (e is locally constant, so translation by e is holomorphic) which we consider as mirror to X with complexified form $B + i\omega$. In this way, Gross manages to match up complexified symplectic deformations of X with complex structures on $\check{X}$.

The 2-Torus

Mirror symmetry is nontrivial even for the simplest Calabi–Yau – the 2-torus. This can be written as an SYZ fibration $T^2 \xrightarrow{\pi} B = S^1$, and write B as $\mathbb{R}/a\mathbb{Z}$ with its standard integral affine structure induced by $\mathbb{Z} \subset \mathbb{R}$. This trivializes $T^*B = B \times \mathbb{R}$ and the lattice Λ in it as $B \times \mathbb{Z} \subset B \times \mathbb{R}$. So as a symplectic manifold,

$$T^2 = \frac{T^*S^1}{\Lambda} = \frac{[0,a] \times [0,1]}{(0,p) \sim (a,p), (q,0) \sim (q,1)} \qquad [8]$$

with symplectic coordinates (q,p) in which the symplectic form is $\omega = \mathrm{d}p \wedge \mathrm{d}q$ (so $\int_{T^2} \omega = a$). Again, the B-field, $b \in H^1(R^1\pi_*\mathbb{R}/\mathbb{Z}) = H^2(T^2, \mathbb{R}/\mathbb{Z})$, is in H^1 of the locally constant sections of the dual fibration.

In our trivialization $B \cong \mathbb{R}/a\mathbb{Z}$, $\Lambda^* \subset TB$ is also standard: $B \times \mathbb{Z} \subset B \times \mathbb{R}$, so the mirror has the same description as in [8] in which the complex structure is standard: $J\partial_p = \partial_q$. That is, $p + \mathrm{i}q$ gives a local holomorphic coordinate.

For nonzero B-field $b \neq 0$, twisting the dual fibration by b gives

$$T^2 = \frac{T^*S^1}{\Lambda} = \frac{[0,a] \times [0,1]}{(0,p) \sim (a, b+p), (q,0) \sim (q,1)} \qquad [9]$$

again with holomorphic structure given by $p + \mathrm{i}q$ and SYZ fibration $\check{\pi}$ being projection onto q. So, as a complex manifold the mirror is $\mathbb{C}$ divided by the lattice

$$\Lambda = \langle 1, b + \mathrm{i}a \rangle$$

Changing b to $b+1$ does not alter this lattice, so the construction is well defined for $b \in \mathbb{R}/\mathbb{Z} \cong H^1(R^1\pi_*\mathbb{R}/\mathbb{Z})$, and we have the standard description of an elliptic curve via its period point $\tau = b + \mathrm{i}a$ in the upper half plane (as $a > 0$). Mirror symmetry has indeed swapped the complexified symplectic parameter $b + \mathrm{i}a = \int_{T^2}(b + \mathrm{i}\omega)$ for the complex structure modulus $\tau = b + \mathrm{i}a$. $\mathrm{SL}(2,\mathbb{Z})$ acts on both sides (in the standard way on τ, and as symplectomorphisms modulo those isotopic to the identity on the A-side) permuting the choices of SYZ fibration. We note that in this case the fibrations are special Lagrangians in the flat metric, with no singular fibers.

Polishchuk and Zaslow have worked out in detail how Kontsevich's conjecture works in this case. The general picture for any torus fibration is an extension of the fiberwise duality that led to SYZ. Namely, Lagrangian multisections L of the fibration, of degree r over the base, give r points on each fiber, and so r flat U(1) connections on the dual fiber. The resulting $\mathrm{U}(1)^{\times r}$ connections can be glued together and twisted by the flat connection on L, to give a rank-r vector bundle with connection on the mirror. Arinkin and Polishchuk show that in general the Lagrangian condition implies the integrability condition $F^{0,2} = 0$ of the resulting connection, giving a holomorphic structure on the bundle. Leung–Yau–Zaslow show that the special Lagrangian condition gives a perturbation of the HYM equations on the connection. Branching of sections has been dealt with by Fukaya, and requires instanton corrections from holomorphic disks. Other Lagrangians with linear intersection with the fibers can be dealt with similarly. T^2 is simpler because all Lagrangians with vanishing Maslov class can be isotoped into straight lines (i.e., sLags in the flat metric) with no branching. The upshot is that the slope of the sLag over the base corresponds to the slope $(\int_{T^2} c_1/\mathrm{rank}) \in [-\infty, \infty]$ of the mirror sheaf.

The Large Complex Structure Limit

The LKLP for T^2 is clearly $\lim a \to \infty$. On the mirror then, the LCLP is at $\tau = b + \mathrm{i}a \to b + \mathrm{i}\infty$, the nodal torus compactifying the moduli of elliptic curves. Metrically, however, in the (Ricci-) flat metric, things look different; if we rescale to have fixed diameter, the torus collapses to the base of its SYZ fibration, and all of its fibers contract. This is an important general feature of the difference between complex and metric descriptions of LCLPs; see the description of the quintic in the next section.

We note that, as in the compactifications discussed in an earlier section, the monodromy around this LCLP is given by rotating the B-field: $b \mapsto b + 1$. This gives back the same elliptic curve, but after a monodromy diffeomorphism T, which, from [9], is seen to be

$$T: q \mapsto q, \; p \mapsto p + q/a$$

On $H^1(T^2) = \mathbb{Z}[\text{fiber}] \oplus \mathbb{Z}[\text{section}]$ this acts as

$$T_* = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \qquad [10]$$

This is called a Dehn twist. Picking the 0-section $O = \{p = 0\}$ in the mirror [9] when $b = 0$, this is taken to the section

$$T(O) = \{p = q/a\}$$

and T is in fact the translation by this section $T(O)$ on T^2, using the group structure on the fibers (now we have chosen a 0-section). Again, Gross (1998) has shown that this is a general feature of LCLPs.

If we pick a Kähler structure on this family of complex tori, T turns out to be a symplectomorphism. Importantly, its mirror is not a holomorphic automorphism, but an equivalence of the derived category of coherent sheaves. As above, the section $T(O)$ corresponds to a slope-one line bundle L on the mirror, and the monodromy action corresponds to

$$\otimes L : D^{\mathrm{b}} \to D^{\mathrm{b}} \qquad [11]$$

on the derived category. Again, this is a more general feature of these LCLPs, with L such that $c_1(L)$ equals the symplectic form which generated

the ray along which the original LKLP was reached. In general, the SYZ fiber is the invariant cycle under T_* [10], and, on the mirror, structure sheaves of points are invariant under $\otimes L$. On the cohomology of T^2, cupping with $\mathrm{ch}(L) = e^{c_1(L)} = 1 + c_1(L)$ has the same action [10] on $H^{\mathrm{ev}} = \mathbb{Z}(c_1(L)) \oplus \mathbb{Z}(1)$.

Notice we have used the choices of fibration and 0-section to produce the equivalence of triangulated categories and to equate the monodromy actions. Kontsevich's conjectural equivalence is not canonical, but is fixed by a choice of fibration and 0-section. In turn, a fibration should be fixed by a choice of LCLP or LKLP from the resulting collapse (in the Ricci-flat metric) onto a half-dimensional S^n base. The choice of 0-section is then rather arbitrary (as monodromy about the LCLP changes it) but determines the equivalence of categories. Different choices of section give different equivalences, differing, for instance, by the monodromy transformation $\otimes L$ [11].

Another point of view is that a Lagrangian fibration and 0-section determine a group structure on the fibers and so on the Fukaya category (translating Lagrangian multisections by multiplication on each fiber). This corresponds to a choice of tensor product on the derived category of the mirror; the identity for this product is then the structure sheaf $\mathcal{O}_X$ mirror to the 0-section, and an ample line bundle is given by the action of the monodromy transformation $L = T(\mathcal{O}_X)$; T then acts as $\otimes T(\mathcal{O}_X)$ [11]. Since X is determined by the graded ring

$$\bigoplus_{j\gg 0} H^0_X(L^j) = \bigoplus_{j\gg 0} \mathrm{Hom}^*(\mathcal{O}_X, T^j(\mathcal{O}_X))$$

one might also try to construct X purely from the 0-section O and LCLP monodromy on $\check{X}$, as

$$X = \mathrm{Proj} \bigoplus_{j\gg 0} HF^*(O, T^j(O))$$

A problem is to show that $\oplus_{j\gg 0} HF^0(O, T^j(O))$ is finitely generated; a related problem is to show that, for $j \gg 0$, the above Floer homologies vanish except for $* = 0$.

We now turn to the quintic 3-folds, where we will see how to identify the (homology classes of the) 0-section and fiber in general using Hodge theory.

The Quintic 3-Fold

The simplest Calabi–Yau 3-fold is given by the zeros Q of a homogeneous quintic polynomial on $\mathbb{P}^4$, that is, an anticanonical divisor of $\mathbb{P}^4$. By adjunction, this has trivial canonical bundle, and so is Calabi–Yau. By the Lefschetz hyperplane theorem, it has $h^{1,1} = 1$, so computing its Euler number to be $e = -200$, we find that $h^{2,1} = 101$ gives its number of complex deformations. Alternatively, this can be seen by showing that all such deformations are themselves quintics, then dividing the 126-dimensional space of quintic polynomials by the 25-dimensional GL $(5, \mathbb{C})$. Thus, its mirror has one complex structure deformation and 101 Kähler classes.

Greene and Plesser prescribed the following mirror. Take the special one-dimensional family of Fermat quintics

$$Q_\lambda = \left\{ \sum_{i=0}^{4} x_i^5 - \lambda \prod_{i=0}^{4} x_i = 0 \right\} \subset \mathbb{P}^4 \qquad [12]$$

with the action of $\{(\alpha_0, \ldots, \alpha_4) \in (\mathbb{Z}/5)^5 : \prod_i \alpha_i = 1\} \cong (\mathbb{Z}/5)^4$ given by rescaling the x_i by fifth roots of unity. Dividing by the diagonal $\mathbb{Z}/5$ projective stabilizer, we get a free $(\mathbb{Z}/5)^3$ action; the mirror of the quintic is any crepant $(K = \mathcal{O})$ resolution of the quotient:

$$\check{Q}_\lambda = \frac{\widehat{Q_\lambda}}{(\mathbb{Z}/5)^3}$$

Different resolutions give different Kähler cones whose union is the moveable cone; its complexification is locally isomorphic to the complex structure moduli space of Q. $h^{1,1}(\check{Q}_\lambda) = 101$ for any crepant resolution, and $h^{2,1}(\check{Q}_\lambda) = 1$ corresponds locally to the one complex structure deformation [12]. In fact, for $\alpha^5 = 1$, multiplying x_0 by α shows that $\check{Q}_\lambda \cong \check{Q}_{\alpha\lambda}$, and λ^5 parametrizes the complex structure moduli.

The LCLP is at $\lambda = \infty$, that is, it is the quotient of the union of hyperplanes

$$Q_\infty = \left\{ \prod_{i=0}^{4} x_i = 0 \right\} = \{x_0 = 0\} \cup \cdots \cup \{x_4 = 0\} \qquad [13]$$

This is a union of toric varieties, each with a T^3 action inherited from the toric T^4 action on $\mathbb{P}^4$. Much more generally, Batyrev's construction considers the anticanonical divisors (and even more generally, complete intersections) in toric varieties fibered over the boundary of the moment polytope, and takes as mirror the anticanonical divisor of the toric variety associated to the dual polytope. However, most of the geometry is visible in this quintic example.

Equation [13] is the analog of the nodal torus of the last section, and we emphasize again that metrically it looks nothing like this; the Ricci-flat metric collapses the T^3 toric fibers to the base S^3 (with a singular metric). General LCLPs look rather similar,

with such "as bad as possible" normal crossing singularities. Smoothing a local model (in $x_0 = 1$) $\prod_{i=1}^4 x_i = 0$, we can see the tori in $\{\prod_{i=1}^4 x_i = \epsilon\}$:

$$T^3 = \left\{ |x_1| = \delta_1, |x_2| = \delta_2, |x_3| = \delta_3, x_4 = \frac{\epsilon}{x_1 x_2 x_3} \right\} \qquad [14]$$

These are even Lagrangian in the standard symplectic form on the local model, and fiber the smoothing over the base $\{(\delta_1, \delta_2, \delta_3)\}$. It turns out that, metrically, these tori (which vanish into the normal crossings singularity at the LCLP) actually form a large part of the smooth Calabi–Yau. This enlightens the apparent paradox between the SYZ conjecture and the Batyrev construction, that is, why a vertex of the original moment polytope (corresponding to the deepest type of singularity $(0,0,0,0) \in \{\prod_{i=1}^4 x_i = 0\}$) can be replaced by the dual three-dimensional face in the dual polytope. This was first suggested by Leung and Vafa.

Gross and Siebert (2003) exploit this to extend SYZ and Batyrev's construction to nontoric LCLP Calabi-Yau manifolds; it is only the local toric nature of the normal crossing singularities of the LCLP that they use. It seems possible that their construction will give the mirrors of all Calabi–Yau manifolds with LCLPs. Much of mirror symmetry should soon be reduced to graphs (the discriminant locus of a Lagrangian torus fibration) in spheres, and further graphs over which D-branes (such as holomorphic curves) fiber, as in recent conjectures of Kontsevich and Soibelman and Fukaya (2005). It may soon be possible to write down a triangulated category in terms of such data. The full geometric story (involving Joyce's description of sLag fibrations, for instance) is still some way off, however; we cannot even write down an explicit Ricci-flat metric on a compact Calabi–Yau.

Monodromy around the LCLP

As well as the SYZ torus fiber [14] we can also see a Lagrangian 0-section on the quintic and its mirror as a component of the real locus of [12] for $\lambda > 5$. Remarkably, like the torus [14], this cycle was already described and used by Candelas *et al.* (1991), long before the relevance of torus fibrations was suspected.

Gross and Ruan have been able to describe the quintic and its mirror (at least topologically or symplectically) very explicitly as a simple torus fibration over this S^3 with a natural integral affine structure and codimension-two graph discriminant locus (see, e.g., Gross *et al.* (2003)).

Under monodromy about $\lambda = \infty$, the 0-section is moved to another section $T(O)$, and T is given by translation by $T(O)$ using the group structure on the fibers. This is the analog of the Dehn twist [10], and one can choose a basis of $H_3(\check{Q})$ (with first element the invariant cycle, the T^3-fiber, second element a cycle fibered over a curve in S^3, third fibered over a surface, and last the 0-section itself) such that

$$T_* = \begin{pmatrix} 1 & 1 & * & * \\ 0 & 1 & * & * \\ 0 & 0 & 1 & * \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad [15]$$

Like the Dehn twist [10], it turns out that T_* is maximally unipotent; that is, we have in n-dimensions,

$$(T_* - 1)^{n+1} = 0 \quad \text{but} \quad (T_* - 1)^n \neq 0$$

Again, this is a general feature of LCLPs as formulated by Morrison (1993) as part of the definition.

This should be compared with the Lefschetz operator $L = \cup\, \omega$ on the cohomology of the mirror, which also satisfies $L^n \neq 0$, $L^{n+1} = 0$ (or, more relevantly, $\exp(L)$, which satisfies $(e^L - 1)^n \neq 0$, $(e^L - 1)^{n+1} = 0$). Their similarity was noticed by the Griffiths school working on VHS in the late 1960s! Now we know that for Calabi–Yau manifolds at an LCLP dual to an LKLP along a ray $\omega = c_1(L)$ on the mirror, they should be considered mirror operators (up to some factors of the Todd class of the underlying Calabi–Yau, to do with the relationship between the Chern character e^ω of the line bundle L (see [11]) and the Riemann–Roch formula).

Both, by linear algebra of the nilpotent operator $N = \log T_* = \sum_{k=1}^n (T_* - 1)^k$, induce a natural filtration $W_\bullet : 0 \leq W_0 \leq \cdots \leq W_{2n} = H$ on the cohomology on which they operate (which is $H = H^n$ for $N = \log T_*$ and $H = H^{\mathrm{ev}}$ for $N = L = \cup\, \omega$):

$$\begin{aligned} 0 &\leq \operatorname{im}(N^n) \leq \operatorname{im}(N^{n-1}) \cap \ker(N) \leq \cdots \\ &\leq \ker(N^{n-1}) + \operatorname{im}(N) \leq \ker(N^n) \leq H \end{aligned} \qquad [16]$$

For a discussion of the construction of this monodromy weight filtration, the reader is referred to the further reading section. It plays a key role in studying degenerations of varieties and Hodge structures, in this case as we approach the LCLP. It is a beautiful result of Gross that this filtration coincides with the Leray filtration on H^n induced by the fibration. That is, under Poincaré duality, the weight filtration on cycles is by the minimal dimension (over all homologous cycles) of the image in the base over which the cycle is fibered. So, the first graded piece is spanned by the invariant cycle, the T^3 fiber, supported over a point, and the last by the 0-section; cf. [15]. (Similarly on the mirror, the filtration for the Lefschetz operator $\cup e^\omega$ has first piece spanned by the cohomology class of a

point, which is invariant under the monodromy action $\otimes L$ of [11], etc.)

Letting γ_0 be the class of a fiber and γ_1 span W_2/W_0 (which is one-dimensional) over the integers, then $T_*\gamma_1 = \gamma_1 + \gamma_0$. It follows that

$$q = \exp\left(2\pi i \frac{\int_{\gamma_1} \Omega}{\int_{\gamma_0} \Omega}\right)$$

is invariant under monodromy. This is the higher-dimensional analog of the coordinate $\exp(2\pi i\tau)$ on the moduli space of elliptic curves, where τ is the period point. It is this coordinate q that is mirror to the coordinate

$$\int_{\text{line}} \omega$$

on the Kähler moduli space on the mirror quintic, which allows one to compute the correspondence between VHS and Gromov–Witten invariants mentioned in the introduction.

More generally, following Morrison (1993), one can make a rigorous definition of an LCLP using features noted above extended to the case of $h^{2,1} > 0$ (see, e.g., Cox and Katz (1999). Roughly, the upshot is that $\mathcal{M}_{\check{X}}$ (of dimension $s = h^{2,1}(\check{X})$) should be compactified with s divisors $(D_i)_{i=1}^s$ (parametrizing singular varieties) forming a normal crossings divisor meeting at the LCLP, with monodromies T_i about them. There should be a unique (up to multiples) integral cycle γ_0 (our torus fiber) invariant under all T_i, and cycles $(\gamma_i)_{i=1}^s$ such that

$$\tau_i = \frac{\int_{\gamma_i} \Omega}{\int_{\gamma_0} \Omega}$$

is logarithmic at D_i; that is $\tau_i = (1/(2\pi i)) \log(z_i)$, where z_i is a local parameter for $D_i = \{z_i = 0\}$.

So, $z_i = \exp(2\pi i\tau_i)$ form local coordinates for moduli space, mirror to the polydisk coordinates [2] on $\mathcal{K}_X^{\mathbb{C}}$. The direction of approach to the LKLP in that section corresponds to the holomorphic curve $z_i^{k_i} = z_j^{k_i}$ [3] we take through the LCLP ($z_i = 0\,\forall i$), and the monodromy $\sum N_i T_i$ varies accordingly, but the corresponding weight filtration $W_\bullet$ remains constant if $k_i \neq 0\,\forall i$, by a theorem of Cattani and Kaplan.

Morrison then requires that the $(\gamma_i)_{i=0}^s$ should form an integral basis for $W_2 = W_3$ (with γ_0 a basis of $W_0 = W_1$). Finally, part definition and part conjecture, we should be able to make a choice such that they satisfy the condition $\log T_i(\gamma_j) = \delta_{ij}\gamma_0$.

Of course, as has been emphasized, Morrison's definition of an LCLP is really where the mathematics and geometry of mirror symmetry begin, and should have been the starting point of this article. But that would have required appreciable knowledge of abstract VHS that are best understood, in this context, through the new geometry of Lagrangian torus fibrations that mirror symmetry has inspired.

See also: AdS/CFT Correspondence; Calibrated Geometry and Special Lagrangian Submanifolds; Derived Categories; Fourier–Mukai Transform in String Theory; Geometric Analysis and General Relativity; Geometric Flows and the Penrose Inequality; Geometric Measure Theory; Geometric Phases; Number Theory in Physics; Riemann Surfaces; Several Complex Variables: Compact Manifolds; Topological Gravity, Two-Dimensional; Topological Sigma Models; WDVV Equations and Frobenius Manifolds.

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Modular Tensor Categories *see* Braided and Modular Tensor Categories

Moduli Spaces: An Introduction

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The concept of a moduli space has been used by mathematicians for nearly 150 years, although it was not until the 1960s that Mumford (1965) gave precise definitions of moduli spaces and methods for constructing them. The use of the word "moduli" in this context goes back to Riemann in a paper of 1857, in which he observed that an isomorphism class of compact Riemann surfaces of genus g "hängt ... von $3g-3$ stetig veränderlichen Grössen ab, welche die Moduln dieser Klasse genannt werden sollen." The idea of moduli as parameters in some sense measuring or describing the variation of geometric objects has been of fundamental importance in geometry ever since.

Moduli spaces arise naturally in classification problems in geometry, particularly in algebraic geometry (Mumford 1965, Newstead 1978, Popp 1977, Seshadri 1975, Sundaramanan 1980, Viehweg 1995). Algebraic geometry is, roughly speaking, the study of solutions of systems of polynomial equations in many variables; the solutions to such a system form an algebraic variety. A simple example of an algebraic variety is a hypersurface, consisting of the solutions to a single polynomial equation in some number of variables. We can try to classify hypersurfaces by their degree and their dimension; these are "discrete invariants" for the classification problem, but of course they do not determine hypersurfaces completely, even if we regard two hypersurfaces as equivalent when one is obtained from the other after making a change of coordinates. It is typical of classification problems in algebraic geometry (and other areas of geometry) that there are not enough discrete invariants to classify objects sufficiently finely, and this is where the concept of a moduli space arises.

In complex algebraic geometry, discrete invariants often come from topology. For example, a nonsingular complex curve (i.e., a complex algebraic variety which is a connected complex manifold of dimension 1, in other words a Riemann surface) which is projective (i.e., points have been added at infinity to make it compact) is topologically just a sphere with a number of handles attached to it; the number of handles is called the genus of the curve and is a discrete invariant. Nonsingular complex projective curves (or equivalently compact Riemann surfaces) are not classified completely by their genus g; they are determined by g when regarded simply as topological surfaces, but the genus does not determine their complex structure when $g > 0$.

A classification problem such as this one (the classification of nonsingular complex projective curves up to isomorphism, or, equivalently, compact Riemann surfaces up to biholomorphism), can be resolved into two basic steps.

Step 1 is to find as many discrete invariants as possible (in the case of nonsingular complex projective curves the only discrete invariant is the genus).

Step 2 is to fix the values of all the discrete invariants and try to construct a "moduli space"; that is, a complex manifold (or an algebraic variety) whose points correspond in a natural way to the equivalence classes of the objects to be classified.

What is meant by "natural" here can be made precise (as we shall see shortly) given suitable notions of families of objects parametrized by base spaces and of equivalence of families. A "fine moduli space" is then a base space for a universal family of the objects to be classified (any family is equivalent to the pullback of the universal family along a unique map into the moduli space). If no universal family exists there may still be a "coarse moduli space" satisfying slightly weaker conditions, which are nonetheless strong enough to ensure that if a moduli space exists it will be unique up to canonical isomorphism.

It is often the case that not even a coarse moduli space will exist. Typically, particularly "bad" objects must be left out of the classification in order for a moduli space to exist. For example, a coarse moduli space of nonsingular complex projective curves exists (although to have a fine moduli space we must give the curves some extra structure, such as a level structure), but if we want to include singular curves (which is often important so that we can understand how nonsingular curves can degenerate to singular ones) we must leave out the so-called "unstable curves" to get a moduli space. However all nonsingular curves are stable, so the moduli space of stable curves of genus g is then a compactification of the moduli space of nonsingular projective curves of genus g.

Moduli spaces are often constructed and studied as orbit spaces for group actions (using Mumford's geometric invariant theory or more recently ideas due to Kollár (1997) and Keel and Mori (1997); geometric invariant theoretic quotients can also often be described

naturally as symplectic reductions, and it is in this guise that many moduli spaces in physics appear. Another technique involves period maps, Torelli theorems and variations of Hodge structures, initiated by Griffiths (1984) and others. In the special case of moduli spaces of compact Riemann surfaces, Teichmüller theory can also be used (see e.g., Lehto (1987)).

Remark 1 Recall that a compact Riemann surface (i.e., a compact complex manifold of complex dimension 1) can be thought of as a nonsingular complex projective curve, in the sense that every compact Riemann surface can be embedded in some complex projective space

$$\mathbb{P}_n = \mathbb{C}^{n+1} - \{0\}/(\text{multiplication by nonzero complex scalars})$$

as the solution space of a set of homogeneous polynomial equations. Moreover, two nonsingular complex projective curves are biholomorphic if and only if they are algebraically isomorphic. So, there is a natural identification between the moduli space of compact Riemann surfaces of genus g up to biholomorphism and the moduli space of nonsingular complex projective curves up to isomorphism.

There are other situations where an "algebraic" moduli space can be naturally identified with the corresponding "complex analytic" moduli space, but this is not always the case. For example, if we consider K3 surfaces (compact complex manifolds of complex dimension 2 with first Betti number and first Chern class both zero), we find that the moduli space of all K3 surfaces has complex dimension 20, whereas the moduli spaces of algebraic K3 surfaces (which have one more discrete invariant, the degree, to be fixed) are 19-dimensional.

This problem of algebraic moduli spaces versus nonalgebraic ones is one reason why the question of classifying n-folds (i.e., compact complex manifolds – or, in the algebraic category, nonsingular projective varieties – of dimension n) becomes much harder when $n > 1$ than in the case $n = 1$ (which is the case of compact Riemann surfaces or nonsingular projective curves). Another difficulty is that families of n-folds can be "blown up" along families of subvarieties to produce ever more complicated families.

Remark 2 Recall that we blow up a complex manifold X along a closed complex submanifold Y by removing the submanifold Y from X and glueing in the projective normal bundle of Y in its place. We get a complex manifold $\tilde{X}$ with a holomorphic surjection $\pi : \tilde{X} \to X$ such that π is an isomorphism over $X - Y$ and if $y \in Y$ then $\pi^{-1}(y)$ is the complex projective space associated to the normal space T_yX/T_yY to Y in X at y. If $X = \mathbb{C}^{n+1}$ and $Y = \{0\}$ and we identify $\mathbb{P}_n$ with the set of one-dimensional linear subspaces of $\mathbb{C}^{n+1}$, then

$$\tilde{X} = \{(v, w) \in \mathbb{C}^{n+1} \times \mathbb{P}_n : v \in w\}$$

with $\pi(v, w) = v$.

Again this problem does not arise when $n = 1$, because blowing up a 1-fold makes no difference unless the 1-fold has singularities (in which case blowing up may help to "resolve" the singularities; for example, when we blow up the origin $\{0\}$ in $\mathbb{C}^2$, then the singular curve C in $\mathbb{C}^2$ defined by $y^2 = x^3 + x^2$ is tranformed into a nonsingular curve $\tilde{C}$ with the origin in C replaced by two points, corresponding to the two complex "tangent directions" in C at 0).

Thus, the classification of n-folds when $n > 1$ requires a preliminary step before there is any hope of carrying out the two steps described above.

Step 0 (the "minimal model programme" of Mori (1987) and others): Instead of all the objects to be classified, consider only specially "good" objects, such that every object is obtained from one of these specially good objects by a sequence of blow-ups (or similar carefully prescribed operations).

How to carry out Mori's minimal model program is well understood for algebraic surfaces and 3-folds, but in higher dimensions is incomplete as yet (Kollár and Mori 1998). We shall ignore both step 0 and step 1 from now on, and concentrate on step 2, the construction of moduli spaces.

Ingredients of a Moduli Problem

Formally before posing a moduli problem, we need to fix the category in which we are working; that is, we need to specify what we mean by "space" and "map" in the description below. If, for example, we are working in complex analytic geometry then we might take "space" to mean a complex manifold (or more generally we might allow singularities) and take "map" to mean a complex analytic map, whereas in algebraic geometry "space" might mean an algebraic variety, or a scheme, or even a stack, with "map" interpreted as a morphism of algebraic varieties (or schemes, or stacks).

Once this is fixed, the ingredients of a moduli problem are:

1. a set A of objects to be classified,
2. an equivalence relation $\sim$ on A,
3. the concept of a family of objects in A with base space S (or parametrized by S), and sometimes
4. the concept of equivalence of families.

These ingredients must satisfy:

1. a family parametrized by a single point $\{p\}$ is just an object in A (and equivalence of objects is equivalence of families over $\{p\}$) and
2. given a family X parametrized by a space S and a map $\phi:\tilde{S} \to S$, there is a family ϕ^*X parametrized by $\tilde{S}$ (the "pullback of X along ϕ"), with pullback being functorial and preserving equivalence.

In particular, for any family X parametrized by S and any $s \in S$, there is an object X_s given by pulling back X along the inclusion of $\{s\}$ in S. We think of X_s as the object in the family X whose parameter is the point s in the base space S.

Example 1 A family of compact Riemann surfaces parametrized by a complex manifold S is a surjective holomorphic map

$$\pi : T \to S$$

from a complex manifold T of (complex) dimension $\dim(T) = \dim(S) + 1$ to S, such that π is proper (i.e., the inverse image $\pi^{-1}(C)$ of any compact subset C of S under π is compact) and has maximal rank (i.e., its derivative is everywhere surjective). Then $\pi^{-1}(s)$ is a compact Riemann surface for each $s \in S$, and is the object in the family with parameter s.

The family defined by π is an algebraic family if π is a morphism of nonsingular complex projective varieties.

Example 2 A family of nonsingular complex projective varieties parametrized by a nonsingular complex variety S is a proper surjective morphism

$$\pi : T \to S$$

with T nonsingular and π having maximal rank. We can also allow T and S to be singular, but then we require an extra technical condition (that π must be flat with reduced fibers).

In the above example, equivalence of families $\pi_1 : T_1 \to S_1$ and $\pi_2 : T_2 \to S_2$ is given by isomorphisms $f : T_1 \to T_2$ and $g : S_1 \to S_2$ such that $g \circ \pi_1 = \pi_2 \circ f$. Equivalence of families in the first example is similar.

Definition 1 A "deformation" of a nonsingular projective variety or compact complex manifold M is given by a family $\pi : T \to S$ together with an isomorphism

$$\pi^{-1}(s_0) \cong M$$

for some $s_0 \in S$.

Strictly speaking, the deformation is the germ at s_0 of such a π; that is, the restriction of π over any open neighborhood of s_0 in S determines the same deformation of M as π does.

A study of deformations leads to information about the local structure of moduli spaces. Let $\pi : X \to S$ be a deformation of a compact complex manifold $M = \pi^{-1}(s_0)$ where $s_0 \in S$. We can cover M (thought of as a subset of X) with open subsets W_i of X such that there exist isomorphisms

$$h_i : W_i \to U_i \times V_i$$

where $V_i = \pi(W_i)$ is open in S and $U_i = M \cap W_i$ is open in $M = \pi^{-1}(s_0)$ and the projection of h_i onto V_i is just $\pi : W_i \to V_i$. For each $i \neq j$, we then get a holomorphic vector field θ_{ij} on $U_i \cap U_j$ by differentiating $h_i \circ h_j^{-1}$ in the direction of any tangent vector $v \in T_{s_0}S$. These holomorphic vector fields define a 1-cocycle in the tangent sheaf Θ of M. This gives us the "Kodaira–Spencer map"

$$\rho_\pi : T_{s_0}S \to H^1(M, \Theta)$$

Theorem 1 (Kuranishi). *If M is a compact complex manifold, then it has a deformation $\pi : X \to S$ with $\pi^{-1}(s_0) = M$ such that*

(i) *the Kodaira–Spencer map $\rho_\pi : T_{s_0}S \to H^1(M, \Theta)$ is an isomorphism,*
(ii) *π has the local universal property for deformations (i.e., any deformation of M is locally the pullback of π along a map f into S),*
(iii) *if $H^0(M, \Theta) = 0$, then the map f in (ii) is unique, and*
(iv) *if $H^2(M, \Theta) = 0$, then S is nonsingular at s_0 and so $\dim S = \dim H^1(M, \Theta)$.*

This deformation π is called the "Kuranishi deformation" of M (its germ at s_0 is unique up to isomorphism), and S is called the "Kuranishi space" of M.

Example 3 A family of holomorphic (or algebraic) vector bundles over a compact Riemann surface (or nonsingular complex projective curve) Σ is a vector bundle over $\Sigma \times S$ where S is the base space (see e.g., Verdier and Le Potier (1985)). A deformation of a vector bundle E_0 over Σ is then given by a vector bundle E over a product $\Sigma \times S$ together with an isomorphism

$$E|_{\Sigma \times \{s_0\}} \cong E_0$$

for some $s_0 \in S$ (strictly speaking it is the germ at s_0 of such a family of vector bundles).

Fine and Coarse Moduli Spaces

For definiteness, except when it is specified otherwise, let us consider moduli problems in algebraic geometry with "space" meaning algebraic variety (over some fixed field k which is usually $\mathbb{C}$) and "map" meaning morphism of algebraic varieties.

Definition 2 A "fine moduli space" for a given (algebro-geometric) moduli problem is an algebraic variety M with a family U parametrized by M having the following (universal) property: for every family X parametrized by a base space S, there exists a unique map $\phi : S \to M$ such that

$$X \sim \phi^* U$$

U is then called a "universal family" for the given moduli problem.

Many moduli problems have no fine moduli space, but nonetheless there may be a moduli space satisfying slightly weaker conditions, called a coarse moduli space. If a fine moduli space does exist, it will automatically satisfy the conditions to be a coarse moduli space. Both fine and coarse moduli spaces, when they exist, are unique up to canonical isomorphism.

Definition 3 A "coarse moduli space" for a given moduli problem is an algebraic variety M with a bijection

$$\alpha : A/{\sim} \to M$$

(where as before A is the set of objects to be classified up to the equivalence relation $\sim$) from the set $A/{\sim}$ of equivalence classes in A to M such that:

(i) For every family X with base space S, the composition of the given bijection $\alpha : A/{\sim} \to M$ with the function

$$\nu_X : S \to A/{\sim}$$

which sends $s \in S$ to the equivalence class $[X_s]$ of the object X_s with parameter s in the family X, is a morphism.

(ii) When N is any other variety with $\beta : A/{\sim} \to N$ such that for each family X parametrized by a base space S the composition $\beta \circ \nu_X : S \to N$ is a morphism, then

$$\beta \circ \alpha^{-1} : M \to N$$

is a morphism.

Remark 3 For some moduli problems, a family X with base space S which is connected and of dimension strictly greater than zero may exist such that for some $s_0 \in S$ we have

(i) $X_s \sim X_t$ for all $s, t \in S - \{s_0\}$ and
(ii) $X_s \not\sim X_{s_0}$ for all $s \in S - \{s_0\}$.

This is the "jump phenomenon," and when it occurs we cannot construct a moduli space including the equivalence class of the object X_{s_0}. Typically, to construct a moduli space, some objects (often called "unstable") must be left out because of the jump phenomenon and we only get a moduli space of "stable" objects. This happens, for example, in the construction of moduli spaces of complex projective curves, if we want to include singular curves, or moduli spaces of vector bundles.

Example 4 The Jacobian $J(\Sigma)$ of a compact Riemann surface Σ is a fine moduli space for holomorphic line bundles (i.e., vector bundles of rank 1) of fixed degree over Σ up to isomorphism. As a complex manifold

$$J(\Sigma) \cong \mathbb{C}^g / \Lambda$$

where g is the genus of Σ and Λ is a lattice of maximal rank in $\mathbb{C}^g$ (in other words $J(\Sigma)$ is a complex torus). Since $J(\Sigma)$ is also a complex projective variety, it is an "abelian variety."

More precisely, $J(\Sigma)$ is the quotient of the complex vector space $H^0(\Sigma, K_\Sigma)$ of dimension g by the lattice $H^1(\Sigma, Z) \cong Z^{2g}$. Here K_Σ is the complex cotangent bundle of Σ and $H^0(\Sigma, K_\Sigma)$ is the space of its holomorphic sections, that is, the space of holomorphic differentials on Σ. If we choose a basis $\omega_1, \ldots, \omega_g$ of holomorphic differentials and a standard basis $\gamma_1, \ldots, \gamma_{2g}$ for $H_1(\Sigma, \mathbb{Z})$ such that

$$\gamma_i . \gamma_{i+g} = 1 = -\gamma_{i+g} . \gamma_i$$

when $1 \le i \le g$ and all other intersection pairings $\gamma_i . \gamma_j$ are zero, then we can associate to Σ the $g \times 2g$ "period matrix" $P(\Sigma)$ given by integrating the holomorphic differentials ω_i around the 1-cycles γ_j. The Jacobian $J(\Sigma)$ can then be identified with the quotient of $\mathbb{C}^g$ by the lattice spanned by the columns of this period matrix.

We can in fact always choose the basis $\omega_1, \ldots, \omega_g$ of holomorphic differentials so that the period matrix $P(\Sigma)$ is of the form

$$(I_g \; Z)$$

where I_g is the $g \times g$ identity matrix. This period matrix is called a "normalized period matrix." The Riemann bilinear relations tell us that Z is symmetric and its imaginary part is positive definite.

Example 5 The moduli space $\mathcal{A}_g$ of all abelian varieties of dimension g was one of the first moduli spaces to be constructed. We have

$$\mathcal{A}_g \cong \mathcal{H}_g/\mathrm{Sp}(2g;\mathbb{Z})$$

where $\mathcal{H}_g$ is Siegel's upper half space, which consists of the symmetric $g \times g$ complex matrices with positive-definite imaginary part.

Example 6 One way to construct and study the moduli space $\mathcal{M}_g$ of compact Riemann surfaces of genus g is via the "Torelli map"

$$\tau : \mathcal{M}_g \to \mathcal{A}_g$$

given by

$$\Sigma \mapsto J(\Sigma)$$

Torelli's theorem tells us that τ is injective (cf. Griffiths (1984)). Describing the image of $\mathcal{M}_g$ in $\mathcal{A}_g$ is known as the Schottky problem.

We can calculate the dimension of the moduli space $\mathcal{M}_g$ using Kuranishi theory as in the previous section: we get

$$\dim \mathcal{M}_g = \dim H^1(\Sigma, \Theta) = 3g - 3$$

for any compact Riemann surface Σ of genus $g \geq 2$. In fact, if M is any compact complex manifold and there exists a fine moduli space of complex manifolds diffeomorphic to M, then the moduli space is locally isomorphic near $[M]$ to the Kuranishi space near s_0. More often, there is only a coarse moduli space (as in the case of $\mathcal{M}_g$), and then the moduli space is locally isomorphic near $[M]$ to the quotient of the Kuranishi space by the action of the group of automorphisms of M.

For the Teichmüller approach to $\mathcal{M}_g$ (cf. Lehto (1987)), we consider the space of all pairs consisting of a compact Riemann surface of genus g and a basis $\gamma_1, \ldots, \gamma_{2g}$ for $H_1(\Sigma, \mathbb{Z})$ as above such that

$$\gamma_i.\gamma_{i+g} = 1 = -\gamma_{i+g}.\gamma_i$$

if $1 \leq i \leq g$ and all other intersection pairings $\gamma_i.\gamma_j$ are zero. If $g \geq 2$, this space (called Teichmüller space) is naturally homeomorphic to an open ball in $\mathbb{C}^{3g-3}$ (by a theorem of Bers). The mapping class group Γ_g (which consists of the diffeomorphisms of the surface modulo isotopy) acts discretely on Teichmüller space, and the quotient can be identified with the moduli space $\mathcal{M}_g$. This gives us a description of $\mathcal{M}_g$ as a complex analytic space, but not as an algebraic variety.

To construct the moduli space $\mathcal{M}_g$ as an algebraic variety, we can use the fact that every compact Riemann surface of genus g can be embedded canonically as a curve of degree $6(g-1)$ in a projective space of dimension $5g-6$. The use of the word "canonical" here is a rather poor pun; it refers both to the canonical line bundle (or cotangent bundle) of the Riemann surface, although here "tricanonical" would be more accurate, and also to the fact that no choices are involved, except that a choice of basis is needed to identify the projective space with the standard one P_{5g-6}. This enables us to identify $\mathcal{M}_g$ with the quotient of an algebraic variety by the group $\mathrm{PGL}(n+1;\mathbb{C})$. However, here we do not have a discrete group action, and to construct the quotient we must use Mumford's geometric invariant theory (see below), which was developed in the 1960s in order to provide algebraic constructions of this moduli space and others.

In fact, geometric invariant theory also provides a beautiful compactification of $\mathcal{M}_g$ known as the Deligne–Mumford (1969) compactification $\bar{\mathcal{M}}_g$. This compactification is itself a moduli space: it is the moduli space of (Deligne–Mumford) stable curves, which are complex projective curves with only nodal singularities and at most finitely many automorphisms. $\bar{\mathcal{M}}_g$ is singular but in a relatively mild way; it is the quotient of a nonsingular variety by a finite group action.

The moduli space $\mathcal{M}_{g,n}$ of nonsingular complex projective curves of genus g with n marked points has a similar compactification $\bar{\mathcal{M}}_{g,n}$ which is the moduli space of complex projective curves with n marked nonsingular points and with only nodal singularities and finitely many automorphisms. Finiteness of the automorphism group of such a curve Σ is equivalent to the requirement that any irreducible component of genus 0 (respectively 1) has at least 3 (respectively 1) special points, where "special" means either marked or singular in Σ.

The construction of $\mathcal{M}_g$ using the period matrices of curves and the Torelli theorem leads to a different compactification $\tilde{\mathcal{M}}_g$ of $\mathcal{M}_g$ known as the Satake (or Satake–Baily–Borel) compactification. Like the Deligne–Mumford compactification, $\tilde{\mathcal{M}}_g$ is a complex projective variety, but the boundary of $\mathcal{M}_g$ in $\tilde{\mathcal{M}}_g$ has (complex) codimension 2 for $g \geq 3$ whereas the boundary Δ of $\mathcal{M}_g$ in $\bar{\mathcal{M}}_g$ has codimension 1. Each of the irreducible components $\Delta_0, \ldots, \Delta_{[g/2]}$ of Δ is the closure of a locus of curves with exactly one node (irreducible curves with one node in the case of Δ_0, and in the case of any other Δ_i the union of two nonsingular curves of genus i and $g-i$ meeting at a single point). The divisors Δ_i meet transversely in $\bar{\mathcal{M}}_g$, and their intersections define a natural decomposition of Δ into connected strata which parametrize stable curves of a fixed topological type.

For a recent guide to many different aspects of the moduli spaces $\mathcal{M}_g$, see Harris and Morrison (1998).

Example 7 Given any nonsingular complex projective variety X, we can study the moduli spaces of maps from curves to X considered by Kontsevich. Intersection theory on these moduli spaces leads to Gromov–Witten theory and the quantum cohomology of X, with many applications, for example, to enumerative geometry (cf. Cox and Katz (1999), Fulton and Pandharipande (1997), Dijkgraaf *et al.* (1995)).

More precisely, if $2g - 2 + n > 0$ then for any $\beta \in H_2(X;\mathbb{Z})$ there is a moduli space $\mathcal{M}_{g,n}(X,\beta)$ of n-pointed nonsingular complex projective curves Σ of genus g equipped with maps $f:\Sigma \to X$ satisfying $f_*[\Sigma] = \beta$. This moduli space has a compactification $\bar{\mathcal{M}}_{g,n}(X,\beta)$ which classifies "stable maps" of type β from n-pointed curves of genus g into X (Fulton and Pandharipande 1997). Here, a map $f:\Sigma \to X$ from an n-pointed complex projective curve Σ satisfying $f_*[\Sigma] = \beta$ is called stable if Σ has only nodal singularities and $f:\Sigma \to X$ has only finitely many automorphisms, or equivalently every irreducible component of Σ of genus 0 (respectively genus 1) which is mapped to a single point in X by f contains at least three (respectively 1) special points. The forgetful map from $\mathcal{M}_{g,n}(X,\beta)$ to $\mathcal{M}_{g,n}$ which sends $[\Sigma, p_1, \ldots, p_n, f:\Sigma \to X]$ to $[\Sigma, p_1, \ldots, p_n]$ extends to a forgetful map $\pi:\bar{\mathcal{M}}_{g,n}(X,\beta) \to \bar{\mathcal{M}}_{g,n}$ which collapses components of Σ with genus 0 and at most two special points.

Of course, when X is itself a single point, $\mathcal{M}_{g,n}(X,\beta)$ and $\bar{\mathcal{M}}_{g,n}(X,\beta)$ are simply the moduli spaces $\mathcal{M}_{g,n}$ and $\bar{\mathcal{M}}_{g,n}$. In general $\bar{\mathcal{M}}_{g,n}(X,\beta)$ has more serious singularities than $\bar{\mathcal{M}}_{g,n}$ and may indeed have many different irreducible components with different dimensions. In spite of this, $\bar{\mathcal{M}}_{g,n}(X,\beta)$ has a "virtual fundamental class" $[\bar{\mathcal{M}}_{g,n}(X,\beta)]^{\text{vir}}$ lying in the expected dimension

$$3g - 3 + n + (1-g)\dim X + \int_\beta c_1(TX)$$

of $\bar{\mathcal{M}}_{g,n}(X,\beta)$. Gromov–Witten invariants (originally developed mainly in the case $g = 0$ when $\bar{\mathcal{M}}_{g,n}(X,\beta)$ is more tractable, but now also studied when $g > 0$) are obtained by evaluating cohomology classes on $\bar{\mathcal{M}}_{g,n}(X,\beta)$ against this virtual fundamental class.

Moduli Spaces as Orbit Spaces

Example 8 As a simple example, let us consider the moduli space of "hyperelliptic" curves of genus g. By a hyperelliptic curve of genus g, we mean a nonsingular complex projective curve C with a double cover $f: C \to \mathbb{P}_1$ branched over $2g+2$ points in the complex projective line $\mathbb{P}_1$.

Let S be the set of unordered sequences of $2g+2$ distinct points in $\mathbb{P}_1$, which we can identify with an open subset of the complex projective space $\mathbb{P}_{2g+2}$ by associating to an unordered sequence $a_1, \ldots, a_{2g+2}$ of points in $\mathbb{P}_1$ the coefficients of the polynomial whose roots are $a_1, \ldots, a_{2g+2}$. Then, it is not hard to construct a family $\mathcal{X}$ of hyperelliptic curves of genus g with base space S such that the curve parametrized by $a_1, \ldots, a_{2g+2}$ is a double cover of $\mathbb{P}_1$ branched over $a_1, \ldots, a_{2g+2}$. This family is not quite a universal family, but it does have the following two properties.

(i) The hyperelliptic curves $\mathcal{X}_s$ and $\mathcal{X}_t$ parametrized by elements s and t of the base space S are isomorphic if and only if s and t lie in the same orbit of the natural action of $G = \mathrm{SL}(2;\mathbb{C})$ on S.
(ii) (Local universal property) Any family of hyperelliptic curves of genus g is locally equivalent to the pullback of $\mathcal{X}$ along a morphism to S.

These properties (i) and (ii) imply that a (coarse) moduli space M exists if and only if there is an "orbit space" for the action of G on S (Newstead 1978). Here, by an orbit space we mean a G-invariant morphism $\phi: S \to M$ such that every other G-invariant morphism $\psi: S \to M$ factors uniquely through ϕ, and moreover $\phi^{-1}(m)$ is a single G-orbit for each $m \in M$. (We can think of an orbit space as the set of G-orbits endowed in a natural way with the structure of an algebraic variety.)

This sort of situation arises quite often in moduli problems, and the construction of a moduli space is then reduced to the construction of an orbit space. Unfortunately, such orbit spaces do not in general exist. The main problem (which is closely related to the jump phenomenon discussed above) is that there may be orbits contained in the closures of other orbits, which means that the natural topology on the set of all orbits is not Hausdorff, so this set cannot be endowed naturally with the structure of a variety. This is the situation the geometric invariant theory of Mumford (1965) attempts to deal with, telling us how to throw out certain "unstable" orbits in order to be able to construct an orbit space. For more general constructions of orbit spaces which can be used for moduli problems where geometric invariant theory may not be of use, see Keel and Mori (1997) and Kollár (1997).

Example 9 Let $G = \mathrm{SL}(2;\mathbb{C})$ act on $(\mathbb{P}_1)^4$ via Möbius transformations on the Riemann sphere

$$\mathbb{P}_1 = \mathbb{C} \cup \{\infty\}$$

Then,

$$\{(x_1, x_2, x_3, x_4) \in (\mathbb{P}_1)^4 : x_1 = x_2 = x_3 = x_4\}$$

is a single orbit which is contained in the closure of every other orbit. On the other hand, the open subset

$$\{(x_1, x_2, x_3, x_4) \in (\mathbb{P}_1)^4 : x_1, x_2, x_3, x_4 \text{ distinct}\}$$

of $(\mathbb{P}_1)^4$ has an orbit space which can be identified with

$$\mathbb{P}_1 - \{0, 1, \infty\}$$

via the cross ratio.

In order to describe Mumford's geometric invariant theory, let X be a complex projective variety (i.e., a subset of a complex projective space defined by the vanishing of homogeneous polynomial equations), and let G be a complex reductive group acting on X. We also require a "linearization" of the action; that is, an ample line bundle L on X and a lift of the action of G to L. We lose very little generality in assuming that for some projective embedding $X \subseteq \mathbb{P}_n$ the action of G on X extends to an action on $\mathbb{P}_n$ given by a representation

$$\rho : G \to \mathrm{GL}(n+1)$$

and taking for L the hyperplane line bundle on $\mathbb{P}_n$. Algebraic geometry associates to $X \subseteq \mathbb{P}_n$ its homogeneous coordinate ring

$$A(X) = \bigoplus_{k \geq 0} H^0(X, L^{\otimes k}) = \mathbb{C}[x_0, \ldots, x_n]/\mathcal{I}_X$$

which is the quotient of the polynomial ring $\mathbb{C}[x_0, \ldots, x_n]$ in $n+1$ variables by the ideal $\mathcal{I}_X$ generated by the homogeneous polynomials vanishing on X. Since the action of G on X is given by a representation $\rho : G \to \mathrm{GL}(n+1)$, we get an induced action of G on $\mathbb{C}[x_0, \ldots, x_n]$ and on $A(X)$, and we can therefore consider the subring $A(X)^G$ of $A(X)$ consisting of the elements of $A(X)$ left invariant by G. This subring $A(X)^G$ is a graded complex algebra, and because G is reductive it is finitely generated (Mumford 1965). To any finitely generated graded complex algebra we can associate a complex projective variety, and so we can define $X//G$ to be the variety associated to the ring of invariants $A(X)^G$. The inclusion of $A(X)^G$ in $A(X)$ defines a "rational" map ϕ from X to $X//G$, but because there may be points of $X \subseteq \mathbb{P}_n$ where every G-invariant polynomial vanishes, this map will not in general be well defined everywhere on X (i.e., it will not be a morphism).

We define the set X^{ss} of "semistable" points in X to be the set of those $x \in X$ for which there exists some $f \in A(X)^G$ not vanishing at x. Then, the rational map ϕ restricts to a surjective G-invariant morphism from the open subset X^{ss} of X to the quotient variety $X//G$. However, $\phi : X^{ss} \to X//G$ is still not in general an orbit space: when x and y are semistable points of X, we have $\phi(x) = \phi(y)$ if and only if the closures $\overline{O_G(x)}$ and $\overline{O_G(y)}$ of the G-orbits of x and y meet in X^{ss}. Topologically, $X//G$ is the quotient of X^{ss} by the equivalence relation for which x and y in X^{ss} are equivalent if and only if $\overline{O_G(x)}$ and $\overline{O_G(y)}$ meet in X^{ss}.

We define a "stable" point of X to be a point x of X^{ss} with a neighbourhood in X^{ss} such that every G-orbit meeting this neighborhood is closed in X^{ss}, and is of maximal dimension equal to the dimension of G. If U is any G-invariant open subset of the set X^s of stable points of X, then $\phi(U)$ is an open subset of $X//G$ and the restriction $\phi|_U : U \to \phi(U)$ of ϕ to U is an orbit space for the action of G on U in the sense described above, so that it makes sense to write U/G for $\phi(U)$. In particular, there is an orbit space X^s/G for the action of G on X^s, and $X//G$ can be thought of as a compactification of this orbit space.

$$\begin{array}{ccccc} X^s & \underset{\text{open}}{\subseteq} & X^{ss} & \underset{\text{open}}{\subseteq} & X \\ \downarrow & & \downarrow & & \\ X^s/G & \underset{\text{open}}{\subseteq} & X^{ss}/\sim & = & X//G \end{array}$$

Example 10 Let us return to hyperelliptic curves of genus g. We have seen that the construction of a moduli space reduces to the construction of an orbit space for the action of $G = \mathrm{SL}(2; \mathbb{C})$ on an open subset S of $\mathbb{P}_{2g+2}$. If we identify $\mathbb{P}_{2g+2}$ with the space of unordered sequences of $2g+2$ points in $\mathbb{P}_1$, then S is the subset consisting of unordered sequences of distinct points. When the action of G on $\mathbb{P}_{2g+2}$ is linearized in the obvious way, then an unordered sequence of $2g+2$ points in $\mathbb{P}_1$ is semistable if and only if at most $g+1$ of the points coincide anywhere on $\mathbb{P}_1$, and is stable if and only if at most g of the points coincide anywhere on $\mathbb{P}_1$ (cf. Kirwan (1985), chapter 16). Thus, S is an open subset of $\mathbb{P}^s_{2g+2}$, so an orbit space S/G exists with compactification the projective variety $\mathbb{P}_{2g+2}//G$. This orbit space is then the moduli space of hyperelliptic curves of genus g.

Other moduli spaces (such as moduli spaces of curves and of vector bundles; see e.g., Donaldson (1984), Gieseker (1983), Mumford (1965, 1977), and Newstead (1978)) can be constructed as orbit spaces via geometric invariant theory in a similar way.

Symplectic Reduction and Moduli Spaces of Vector Bundles

Geometric invariant theoretic quotients are closely related to the process of reduction in symplectic geometry, and thus many moduli spaces can be described as symplectic reductions.

Suppose that a compact, connected Lie group K with Lie algebra $\boldsymbol{k}$ acts smoothly on a symplectic manifold X and preserves the symplectic form ω. Let us denote the vector field on X defined by the infinitesimal action of $a \in \boldsymbol{k}$ by

$$x \mapsto a_x$$

By a moment map for the action of K on X we mean a smooth map

$$\mu : X \to \boldsymbol{k}^*$$

which satisfies

$$\mathrm{d}\mu(x)(\xi).a = \omega_x(\xi, a_x)$$

for all $x \in X$, $\xi \in T_xX$ and $a \in \boldsymbol{k}$. In other words, if $\mu_a : X \to \mathbb{R}$ denotes the component of μ along $a \in \boldsymbol{k}$ defined for all $x \in X$ by the pairing

$$\mu_a(x) = \mu(x).a$$

between $\mu(x) \in \boldsymbol{k}^*$ and $a \in \boldsymbol{k}$, then μ_a is a Hamiltonian function for the vector field on X induced by a. We shall assume that all our moment maps are equivariant moment maps; that is, $\mu : X \to \boldsymbol{k}^*$ is K-equivariant with respect to the given action of K on X and the co-adjoint action of K on $\boldsymbol{k}^*$.

It follows directly from the definition of a moment map $\mu : X \to \boldsymbol{k}^*$ that if the stabilizer K_ζ of any $\zeta \in \boldsymbol{k}^*$ acts freely on $\mu^{-1}(\zeta)$, then $\mu^{-1}(\zeta)$ is a submanifold of X and the symplectic form ω induces a symplectic structure on the quotient $\mu^{-1}(\zeta)/K_\zeta$. With this symplectic structure, the quotient $\mu^{-1}(\zeta)/K_\zeta$ is called the Marsden–Weinstein reduction, or symplectic quotient, at ζ of the action of K on X. We can also consider the quotient $\mu^{-1}(\zeta)/K_\zeta$ when the action of K_ζ on $\mu^{-1}(\zeta)$ is not free, but in this case it is likely to have singularities.

Example 11 Consider the cotangent bundle T^*Y of any n-dimensional manifold Y with its canonical symplectic form ω which is given by the standard symplectic form

$$\omega = \sum_{j=1}^{n} \mathrm{d}p_j \wedge \mathrm{d}q_j \qquad [1]$$

with respect to any local coordinates $(q_1, \ldots, q_n)$ on Y and the induced coordinates $(p_1, \ldots, p_n)$ on its cotangent spaces. If Y is the configuration space of a classical mechanical system, then T^*Y is the phase space of the system and the coordinates $p = (p_1, \ldots, p_n) \in T*_q Y$ are traditionally called the momenta of the system.

If Y is acted on by a Lie group K, the induced action on T^*Y preserves ω and there is a moment map $\mu : T^*Y \to \boldsymbol{k}^*$ whose components μ_a along $a \in \boldsymbol{k}$ are given by pairing the moment coordinates p with the vector fields on X induced by the infinitesimal action of K; that is,

$$\mu_a(p, q) = p.a_q$$

for all $q \in Y$ and $p \in T_qY$. When $K = \mathrm{SO}(3)$ acts by rotations on $Y = \mathbb{R}^3$, then μ is the angular momentum, or moment of momentum, about the origin.

The connection with geometric invariant theory arises as follows. Let X be a nonsingular complex projective variety embedded in complex projective space $\mathbb{P}_n$, and let G be a complex Lie group acting on X via a complex linear representation $\rho : G \to \mathrm{GL}(n+1; \mathbb{C})$. A necessary and sufficient condition for G to be reductive is that it is the complexification of a maximal compact subgroup K (e.g., $G = \mathrm{GL}(m; \mathbb{C})$ is the complexification of the unitary group $\mathrm{U}(m)$). By an appropriate choice of coordinates on $\mathbb{P}_n$, we may assume that ρ maps K into the unitary group $\mathrm{U}(n+1)$. Then, the action of K preserves the Fubini–Study form ω on $\mathbb{P}_n$, which restricts to a symplectic form on X. There is a moment map $\mu : X \to \boldsymbol{k}^*$ defined (up to multiplication by a constant scalar factor depending on differences in convention on the normalization of the Fubini–Study form) by

$$\mu(x).a = \frac{\overline{\hat{x}}^t \rho_*(a)\hat{x}}{2\pi \mathrm{i} \|\hat{x}\|^2} \qquad [2]$$

for all $a \in \boldsymbol{k}$, where $\hat{x} \in \mathbb{C}^{n+1} - \{0\}$ is a representative vector for $x \in \mathbb{P}_n$ and the representation $\rho : K \to \mathrm{U}(n+1)$ induces $\rho_* : \boldsymbol{k} \to \boldsymbol{u}(n+1)$ and dually $\rho^* : \boldsymbol{u}(n+1)^* \to \boldsymbol{k}^*$.

In this situation, we have two possible quotient constructions, giving us the geometric invariant theory quotient $X//G$ if we want to work in algebraic geometry and the symplectic reduction $\mu^{-1}(0)/K$ if we want to work in symplectic geometry. In fact, these give us the same quotient space, at least up to homeomorphism (and diffeomorphism away from the singularities). More precisely, any $x \in X$ is semistable if and only if the closure of its G-orbit meets $\mu^{-1}(0)$, and the inclusion of $\mu^{-1}(0)$ into X^{ss} induces a homeomorphism

$$\mu^{-1}(0)/K \to X//G$$

There are other quotient constructions closely related to symplectic reduction and geometric invariant

theory, which are useful when working with Kähler or hyper-Kähler manifolds.

In physics, moduli spaces are often described as symplectic reductions of infinite-dimensional symplectic manifolds by infinite-dimensional groups (although the moduli spaces themselves are usually finite-dimensional). One example is given by moduli spaces of holomorphic vector bundles, which can also be described using Yang–Mills theory (cf. Atiyah and Bott (1982)).

The Yang–Mills equations arose in physics as generalizations of Maxwell's equations. They have become important in differential and algebraic geometry formulated over arbitrary compact oriented Riemannian manifolds, and in particular over compact Riemann surfaces and higher dimensional Kähler manifolds. The fundamental theorem of Donaldson, Uhlenbeck, and Yau that a holomorphic bundle over a compact Kähler manifold admits an irreducible Hermitian Yang–Mills connection if and only if it is stable can be thought of as an infinite-dimensional illustration of the link between symplectic reduction and geometric invariant theory.

Let M be a compact oriented Riemannian manifold and let E be a fixed complex vector bundle over M with a Hermitian metric. Recall that a connection A on E (or equivalently on its frame bundle) can be defined by a covariant derivative $d_A : \Omega^p_M(E) \to \Omega^{p+1}_M(E)$, where $\Omega^p_M(E)$ denotes the space of C^∞-sections of $\bigwedge^p T^*M \otimes E$ (i.e., the space of p-forms on M with values in E). This covariant derivative satisfies the extended Leibniz rule

$$d_A(\alpha \wedge \beta) = (d_A\alpha) \wedge \beta + (-1)^p \alpha \wedge d_A\beta$$

for $\alpha \in \Omega^p_M(E), \beta \in \Omega^q_M(E)$, and therefore is determined by its restriction $d_A : \Omega^0_M(E) \to \Omega^1_M(E)$. The Leibniz rule implies that the difference of two connections is given by an $E \otimes E^*$-valued 1-form on M, and hence that the space of all connections on E is an infinite-dimensional affine space $\mathcal{A}$ based on the vector space $\Omega^1_M(E \otimes E^*)$. Similarly, the space of all unitary connections on E (i.e., connections compatible with the Hermitian metric on E) is an infinite-dimensional affine space based on the space of 1-forms with values in the bundle $\mathbf{g}_E$ of skew-adjoint endomorphisms of E. The Leibniz rule also implies that the composition $d_A \circ d_A : \Omega^0_M(E) \to \Omega^2_M(E)$ commutes with multiplication by smooth functions, and thus we have

$$d_A \circ d_A(s) = F_A s$$

for all C^∞ sections s of E, where $F_A \in \Omega^2_M(\mathbf{g}_E)$ is defined to be the curvature of the unitary connection A. The Yang–Mills functional on the space $\mathcal{A}$ of all unitary connections on E is defined as the L^2-norm square of the curvature, given by the integral over M of the product of the function $\|F_A\|^2$ and the volume form on M defined by the Riemannian metric and the orientation. The Yang–Mills equations are the Euler–Lagrange equations for this functional, given by

$$d_A * F_A = 0$$

where d_A has been extended in a natural way to $\Omega^*_M(\mathbf{g}_E)$. The gauge group $\mathcal{G}$, that is, the group of unitary automorphisms of E, preserves the Yang–Mills functional and the Yang–Mills equations.

If M is a complex manifold, we can identify the space $\mathcal{A}^{(1,1)}$ of unitary connections on E with curvature of type (1,1) with the space of holomorphic structures on E, by associating to a holomorphic structure $\mathcal{E}$ the unitary connection whose $(0,1)$-component is given by the $\bar{\partial}$-operator defined by $\mathcal{E}$. This space $\mathcal{A}^{(1,1)}$ is an infinite-dimensional complex subvariety of the infinite-dimensional complex affine space $\mathcal{A}$, acted on by the complexified gauge group $\mathcal{G}_c$ (the group of complex C^∞ automorphisms of E), and two holomorphic structures are isomorphic if and only if they lie in the same $\mathcal{G}_c$-orbit.

When (M, ω) is a compact Kähler manifold, there is a $\mathcal{G}$-invariant Kähler form Ω on $\mathcal{A}$ defined by

$$\Omega(\alpha, \beta) = \frac{1}{8\pi^2} \int_M \operatorname{tr}(\alpha \wedge \beta) \wedge \omega^{n-1}$$

where n is the complex dimension of M. The Lie algebra of $\mathcal{G}$ is the space $\Omega^0_M(\mathbf{g}_E)$ of sections of $\mathbf{g}_E$, and there is a moment map $\mu : \mathcal{A} \to (\Omega^0_M(\mathbf{g}_E))^*$ for the action of $\mathcal{G}$ on $\mathcal{A}$ given by the composition of

$$A \mapsto \frac{1}{8\pi^2} F_A \wedge \omega^{n-1} \in \Omega^{2n}_M(\mathbf{g}_E)$$

with integration over M. On $\mathcal{A}^{(1,1)}$ the norm square of this moment map agrees up to a constant factor with the Yang–Mills functional, which is minimized by the Hermitian Yang–Mills connections.

As in the finite-dimensional situation, for a suitable definition of stability, the moduli space of stable holomorphic bundles of topological type E over M (which plays the role of the geometric invariant theory quotient) can be identified with the moduli space of (irreducible) Hermitian Yang–Mills connections on E (which plays the rôle of the symplectic reduction). This was proved in general for vector bundles over compact Kähler manifolds Uhlenbeck and Yau with a different proof for nonsingular complex projective varieties given by Donaldson.

Over a compact Riemann surface M the situation is relatively simple, as all connections on E have curvature of type $(1, 1)$ and so the infinite-dimensional

complex affine space $\mathcal{A}$ can be identified with the space $\mathcal{C}$ of holomorphic structures on E. A moment map for the action of the gauge group on $\mathcal{A}$ is given by assigning to a connection $A \in \mathcal{A}$ its curvature $F_A \in \Omega^2_M(g_E)$, and, after a suitable central constant has been added, the Hermitian Yang–Mills connections are exactly the zeros of the moment map.

A holomorphic bundle $\mathcal{E}$ over a Riemann surface M is stable (respectively semistable) if $\mu(\mathcal{F}) < \mu(\mathcal{E})$ (respectively $\mu(\mathcal{F}) \leq \mu(\mathcal{E})$) for every proper subbundle $\mathcal{F}$ of $\mathcal{E}$, where

$$\mu(\mathcal{F}) = \deg(\mathcal{F})/\mathrm{rank}(\mathcal{F})$$

When the theory of stability of holomorphic vector bundles was first introduced, Narasimhan and Seshadri proved that a holomorphic vector bundle over M is stable if and only if it arises from an irreducible representation of a certain central extension of the fundamental group $\pi_1(M)$. Atiyah and Bott (1982) translated this in terms of connections to show that a holomorphic vector bundle over M is stable if and only if it admits a unitary connection with constant central curvature. They deduced from this the existence of a homeomorphism between the moduli space $\mathcal{M}(n, d)$ of stable bundles of rank n and degree d over M and the moduli space of irreducible connections with constant central curvature on a fixed C^∞ bundle E of rank n and degree d over M.

See also: BF Theories; Calibrated Geometry and Special Lagrangian Submanifolds; Cohomology Theories; Floer Homology; Gauge Theoretic Invariants of 4-Manifolds; Gauge Theory: Mathematical Applications; Geometric Measure Theory; Geometric Phases; Hamiltonian Group Actions; Instantons: Topological Aspects; Intersection Theory; Riemann Surfaces; Several Complex Variables: Basic Geometric Theory; Several Complex Variables: Compact Manifolds; Topological Gravity, Two-Dimensional; WDVV Equations and Frobenius Manifolds.

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Multicomponent Fluids *see* Interfaces and Multicomponent Fluids

Multi-Hamiltonian Systems

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Introduction

Since the late 1970s, a particular attention in the theory of integrability has been payed to systems admitting more than one Hamiltonian representation. The first examples belonged to the class of infinite-dimensional systems (i.e., partial differential equations), like the Korteweg–de Vries (KdV) equation, the Ablowitz–Kaup–Newell–Segur system, and many other soliton equations (*see* Bi-Hamiltonian Methods in Soliton Theory). It was realized soon that finite-dimensional integrable systems are also likely to possess a bi-Hamiltonian representation. Moreover, a geometric setting for the study of bi-Hamiltonian systems was established, with the introduction of the so-called bi-Hamiltonian manifolds. They are Poisson manifolds with an additional Poisson structure, fulfilling a suitable compatibility condition with the initial Poisson bracket. An important program for the study and the classification of (finite-dimensional) bi-Hamiltonian manifolds was started in the 1990s by Gelfand and Zakharevich. They pointed out that the geometry of such manifolds is extremely rich and complicated.

In this article we present the basic facts concerning the bi-Hamiltonian geometry and its relations with the theory of integrable systems, referring to Recursion Operators in Classical Mechanics in this encyclopedia for the connections with separable systems of Jacobi. In the first section we give the definitions of bi-Hamiltonian manifold and bi-Hamiltonian system, and we present some properties of the former. The next section contains three concrete examples (the Euler top, the open Toda lattice, and a stationary KdV flow) and two important classes of bi-Hamiltonian manifolds, both related to Lie algebras. This is followed by a discussion of the iterative construction of first integrals in involution for a given bi-Hamiltonian system. This procedure is particularly efficient in the case of Poisson–Nijenhuis manifolds, that is, those bi-Hamiltonian manifolds whose second Poisson structure can be obtained by composing the first one with a suitable recursion operator.

Bi-Hamiltonian Systems

First of all, we recall some fundamental definitions from the theory of Poisson manifolds, which are the natural setting for the study of Hamiltonian systems. Let M be a finite-dimensional C^∞-differentiable manifold and let $C^\infty(M)$ be the space of C^∞-functions from M to $\mathbb{R}$. A Poisson bracket on M is a skew-symmetric $\mathbb{R}$-bilinear map

$$\{\cdot,\cdot\}: C^\infty(M)\times C^\infty(M)\to C^\infty(M)$$

fulfilling the Jacobi identity

$$\{\{F,G\},H\}+\{\{H,F\},G\}+\{\{G,H\},F\}=0$$

and the Leibniz rule

$$\{FG,H\}=F\{G,H\}+\{F,H\}G$$

A Poisson manifold is a differentiable manifold endowed with a Poisson bracket. Starting from a Poisson bracket, one can introduce a tensor field P of type $(2,0)$, which we consider as a map from T^*M to TM, defined by

$$\langle dG, P\,dF\rangle=\{F,G\}$$

or, using coordinates on M, by $P^{ij}=\{x^i,x^j\}$. This tensor field is called the Poisson tensor associated with $\{\cdot,\cdot\}$. It is skew-symmetric, and its components satisfy the cyclic condition

$$P^{il}\frac{\partial P^{jk}}{\partial x^l}+P^{jl}\frac{\partial P^{ki}}{\partial x^l}+P^{kl}\frac{\partial P^{ij}}{\partial x^l}=0$$

meaning that the Schouten bracket $[P,P]$ vanishes.

On a Poisson manifold, the vector field $X_H=\{H,\cdot\}=P\,dH$ is called the Hamiltonian vector field associated with H. In coordinates, $X_H^j=P^{ij}\partial H/\partial x^i$. The Jacobi identity is equivalent to the statement that the map $H\mapsto X_H$, assigning to a function H its Hamiltonian vector field X_H, is a Lie algebra homomorphism:

$$X_{\{F,G\}}=[X_F,X_G] \qquad [1]$$

A Casimir function is a function H such that $X_H=0$, that is, a function which is in involution with any other function on M. In terms of the Poisson tensor, a Casimir is a function whose differential belongs to the kernel of P.

The most famous class of Poisson manifolds is certainly that of symplectic manifolds. They can be seen as nondegenerate Poisson manifolds. Indeed, if a Poisson tensor P is invertible, then its inverse defines a closed nondegenerate 2-form (i.e., a symplectic form). Moreover, any Poisson manifold turns out to be foliated in symplectic leaves.

Let us introduce now the bi-Hamiltonian manifolds, which can be considered as a geometric setting for the study of integrable Hamiltonian systems. A manifold M endowed with two Poisson brackets, $\{\cdot,\cdot\}$ and $\{\cdot,\cdot\}'$, is said to be bi-Hamiltonian if the brackets are compatible, that is, if any linear combination (with constant coefficients) of them is still a Poisson bracket. Such a linear combination automatically satisfies all properties of a Poisson bracket except the Jacobi identity. This is fulfilled if and only if the following compatibility condition holds:

$$\begin{aligned}&\{F,\{G,H\}\}' + \{H,\{F,G\}\}' + \{G,\{H,F\}\}'\\ &\quad + \{F,\{G,H\}'\} + \{H,\{F,G\}'\}\\ &\quad + \{G,\{H,F\}'\} = 0 \end{aligned} \qquad [2]$$

for any triple (F,G,H) of functions on M. This amounts to saying that the sum of the two Poisson brackets is also a Poisson bracket. In this case the two (compatible) Poisson brackets are said to form a Poisson pair.

There are some interesting equivalent forms of the compatibility condition [2]. First of all, in terms of the components of the Poisson tensors P and P', it reads

$$\begin{aligned}&P^{il}\frac{\partial (P')^{jk}}{\partial x^l} + P^{jl}\frac{\partial (P')^{ki}}{\partial x^l} + P^{kl}\frac{\partial (P')^{ij}}{\partial x^l}\\ &\quad + (P')^{il}\frac{\partial P^{jk}}{\partial x^l} + (P')^{jl}\frac{\partial P^{ki}}{\partial x^l} + (P')^{kl}\frac{\partial P^{ij}}{\partial x^l} = 0\end{aligned}$$

that is, the Schouten bracket $[P,P']$ vanishes. Moreover, if $X_F = P\,\mathrm{d}F$ is the Hamiltonian vector field associated with $F \in C^\infty(M)$ by means of P and $Y_F = P'\,\mathrm{d}F$ is the one obtained by P', the compatibility condition takes the form

$$\begin{aligned}&[X_F, Y_G] + [Y_F, X_G] = X_{\{F,G\}'} + Y_{\{F,G\}}\\ &\quad \forall F,G \in C^\infty(M)\end{aligned} \qquad [3]$$

to be compared with [1]. Moreover, in terms of Lie derivatives we have the equivalent condition

$$L_{X_F}P' + L_{Y_F}P = 0 \quad \forall F \in C^\infty(M) \qquad [4]$$

Now we turn our attention to special vector fields that can be selected on a bi-Hamiltonian manifold M. Let P and P' be the Poisson tensors associated with the (compatible) Poisson brackets of M. A vector field X on M is said to be bi-Hamiltonian if it is Hamiltonian with respect to both Poisson structures, that is, if there exist two functions H_0 and H_1 such that

$$X = P\,\mathrm{d}H_1 = P'\,\mathrm{d}H_0 \qquad [5]$$

We will see in the following that such vector fields are likely to have a number of first integrals in involution, and thus they are good candidates for a geometric description of integrable systems. The next section is devoted to examples of bi-Hamiltonian (and multi-Hamiltonian) systems.

Examples

The first example is the Euler top, that is, free motions of a rigid body with a fixed point. The equations of motion are

$$\dot{\Gamma}_1 = \frac{I_2 - I_3}{I_2 I_3}\Gamma_2\Gamma_3$$

and its cyclic permutations. They define a vector field in $\mathbb{R}^3$, which is well known to be Hamiltonian with respect to the Lie–Poisson structure on the (dual of the) Lie algebra of 3×3 skew-symmetric matrices. This means that

$$\dot{\Gamma}_j = \{H, \Gamma_j\}, \quad j = 1,2,3$$

where

$$H = \frac{1}{2}\left(\frac{\Gamma_1{}^2}{I_1} + \frac{\Gamma_2{}^2}{I_2} + \frac{\Gamma_3{}^2}{I_3}\right)$$

is the kinetic energy and the bracket $\{\cdot,\cdot\}$ is defined by $\{\Gamma_1,\Gamma_2\} = \Gamma_3$ and its cyclic permutations. Another Hamiltonian representation is given by

$$\dot{\Gamma}_j = \{K, \Gamma_j\}', \quad j = 1,2,3$$

where

$$K = \tfrac{1}{2}(\Gamma_1{}^2 + \Gamma_2{}^2 + \Gamma_3{}^2)$$

and the new bracket $\{\cdot,\cdot\}'$ is defined by $\{\Gamma_1,\Gamma_2\}' = -\Gamma_3/I_3$ and its cyclic permutations.Any linear combination of the two brackets has the form of the second one, and it is very easy to show that the Jacobi identity is satisfied for such a bracket. Therefore, the Euler top is a bi-Hamiltonian system. Let us also notice that

$$\{K, \Gamma_j\} = \{H, \Gamma_j\}' = 0, \quad j = 1,2,3$$

that is, K is a Casimir function for the Lie–Poisson bracket and H is a Casimir function for the new Poisson bracket. Hence, we have the following (recursion) relations:

$$\begin{aligned}\{K,\Gamma_j\} &= 0\\ \{H,\Gamma_j\} &= \{K,\Gamma_j\}'\\ 0 &= \{H,\Gamma_j\}'\end{aligned} \qquad [6]$$

From a geometrical point of view, the situation is as follows. The symplectic leaves of $\{\cdot,\cdot\}$ are the level surfaces of K, that is, spheres, while the symplectic

leaves of $\{\cdot,\cdot\}'$ are the ellipsoids $H=$constant. Their intersections are Lagrangian submanifolds for both symplectic leaves (in the compact case they are the Arnol'd–Liouville tori of the integrable systems, that in this case coincide with the trajectories).

Let us consider now the (three-particle) open Toda lattice. It consists in three particles (with masses equal to 1) moving on the line under a nearest-neighbor interaction of exponential type. The Hamiltonian is given by

$$H=\tfrac{1}{2}(p_1{}^2+p_2{}^2+p_3{}^2)+\exp(q_1-q_2)+\exp(q_2-q_3)$$

and the system is of course Hamiltonian with respect to the canonical Poisson structure of $\mathbb{R}^6$,

$$P=\begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

But the Toda vector field can also be written as $P'\,\mathrm{d}K$, where $K=p_1+p_2+p_3$ is the total momentum and

$$P'=\begin{pmatrix} 0 & 1 & 1 & -p_1 & 0 & 0 \\ -1 & 0 & 1 & 0 & -p_2 & 0 \\ -1 & -1 & 0 & 0 & 0 & -p_3 \\ p_1 & 0 & 0 & 0 & \mathrm{e}^{(q_1-q_2)} & 0 \\ 0 & p_2 & 0 & -\mathrm{e}^{(q_1-q_2)} & 0 & \mathrm{e}^{(q_2-q_3)} \\ 0 & 0 & p_3 & 0 & -\mathrm{e}^{(q_2-q_3)} & 0 \end{pmatrix}$$

is a Poisson tensor, which turns out to be compatible with P. The generalization to an arbitrary number of particles is straightforward. Hence, the open Toda lattice is a bi-Hamiltonian system. In the next section we will show that this property can be used to construct a maximal set of integrals of motion for the Toda lattice, which are automatically in involution.

The third example – a stationary reduction of the KdV equation – comes from the field of soliton equations. Let us recall that the first members of the KdV hierarchy are

$$\begin{aligned} \frac{\partial u}{\partial t_1} &= u_x \\ \frac{\partial u}{\partial t_3} &= \tfrac{1}{4}(u_{xxx}-6uu_x)\ \text{(KdV equation)} \\ \frac{\partial u}{\partial t_5} &= \tfrac{1}{16}(u_{xxxxx}-10uu_{xxx} \\ &\quad -20u_xu_{xx}+30u^2u_x) \end{aligned} \qquad [7]$$

It is well known how to find finite-dimensional reductions for the KdV equation, giving rise to explicit solutions. Indeed, the set of singular points of a given vector field of the hierarchy is a finite-dimensional manifold which is invariant under the flows of the other vector fields, due to the fact that the flows commute. The (finite-dimensional) systems obtained by restricting the KdV hierarchy to such invariant manifolds are called the stationary reductions of KdV. Let us consider explicitly the reduction corresponding to the third vector field of the hierarchy. The set of its critical points is given by

$$u_{xxxxx}-10uu_{xxx}-20u_xu_{xx}+30u^2u_x=0 \qquad [8]$$

and its dimension is 5, since we can use the values of u, u_x, u_{xx}, u_{xxx}, and u_{xxxx} at a fixed point x_0 (i.e., the Cauchy data) as global coordinates. For the sake of simplicity, we set

$$\begin{aligned} &u_0=u(x_0), \quad u_1=u_x(x_0), \quad u_2=u_{xx}(x_0) \\ &u_3=u_{xxx}(x_0), \quad u_4=u_{xxxx}(x_0) \end{aligned}$$

In order to compute the reduced equations of the first flow of [7], we have to take its x-derivative and to use the constraint [8] and its differential consequences to eliminate all the derivatives of order higher than 4. We obtain the equations

$$\begin{aligned} &\frac{\partial u_0}{\partial t_1}=u_1,\ \frac{\partial u_1}{\partial t_1}=u_2,\ \frac{\partial u_2}{\partial t_1}=u_3,\ \frac{\partial u_3}{\partial t_1}=u_4 \\ &\frac{\partial u_4}{\partial t_1}=10u_0u_3+20u_1u_2-30u_0{}^2u_1 \end{aligned} \qquad [9]$$

In the same way, for the KdV equation we get

$$\begin{aligned} \frac{\partial u_0}{\partial t_3} &= \tfrac{1}{4}(u_3-6u_0u_1) \\ \frac{\partial u_1}{\partial t_3} &= \tfrac{1}{4}(u_4-6u_0u_2-6u_1{}^2) \\ \frac{\partial u_2}{\partial t_3} &= \tfrac{1}{4}(4u_0u_3+2u_1u_2-30u_0{}^2u_1) \\ \frac{\partial u_3}{\partial t_3} &= \tfrac{1}{4}(4u_0u_4+6u_1u_3+2u_2{}^2 \\ &\quad -30u_0{}^2u_2-60u_0u_1{}^2) \\ \frac{\partial u_4}{\partial t_3} &= \tfrac{1}{4}(10u_1u_4+10u_0{}^2u_3+10u_2u_3 \\ &\quad -100u_0u_1u_2-60u_1{}^3-120u_0{}^3u_1) \end{aligned} \qquad [10]$$

There are two compatible Poisson structures giving a bi-Hamiltonian formulation of both systems. The corresponding Poisson tensors are

$$P=\begin{bmatrix} 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & -2 & 0 & -20u_0 \\ 0 & 2 & 0 & 20u_0 & 20u_1 \\ -2 & 0 & -20u_0 & 0 & -140u_0{}^2-20u_2 \\ 0 & 20u_0 & -20u_1 & 140u_0{}^2+20u_2 & 0 \end{bmatrix}$$

and

$$P' = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 3u_0 & 6u_1 \\ -\frac{1}{2} & 0 & -3u_0 & -3u_1 & -4u_2 - 15u_0^2 \\ 0 & 3u_0 & 0 & u_2 + 15u_0^2 & u_3 + 30u_0u_1 \\ -3u_0 & 3u_1 & -u_2 - 15u_0^2 & 0 & \begin{matrix} u_4 - 40u_0u_2 + \\ 30u_1^2 - 60u_0^3 \end{matrix} \\ -6u_1 & 4u_2 + 15u_0^2 & -u_3 - 30u_0u_1 & \begin{matrix} -u_4 + 40u_0u_2 - \\ 30u_1^2 + 60u_0^3 \end{matrix} & 0 \end{bmatrix}$$

In fact, if we call X_1 and X_3 the vector fields given by [9] and [10], then the following recursion relations hold:

$$\begin{aligned} P\,dH_0 &= 0 \\ X_1 = P\,dH_1 &= P'\,dH_0 \\ X_3 = P\,dH_2 &= P'\,dH_1 \\ 0 &= P'\,dH_2 \end{aligned} \qquad [11]$$

where

$$\begin{aligned} H_0 &= -u_4 + 10u_0u_2 + 5u_1^2 - 10u_0^3 \\ H_1 &= \tfrac{1}{4}(2u_0u_4 - 2u_1u_3 + u_2^2 - 20u_0^2u_2 + 15u_0^4) \\ H_2 &= \tfrac{1}{16}(2u_2u_4 - 6u_0^2u_4 - u_3^2 + 12u_0u_1u_3 \\ &\quad -16u_0u_2^2 - 12u_1^2u_2 + 60u_0^3u_2 - 36u_0^5) \end{aligned}$$

Therefore, the vector fields X_1 and X_3 are bi-Hamiltonian. The geometry of this bi-Hamiltonian manifold is similar to the one of the first example. The symplectic leaves of both Poisson structures have dimension 4, and the Lagrangian foliation (given by the level submanifolds of H_0, H_1, and H_2) is contained in the intersections of such leaves. This Lagrangian foliation is called by Gelfand and Zakharevich the "axis" of the bi-Hamiltonian manifold.

We also notice that the relations [11] can be collected in the statement that the function $H(\lambda) = H_0\lambda^2 + H_1\lambda + H_2$ is a Casimir of the Poisson pencil $P_\lambda = P' - \lambda P$, that is,

$$P_\lambda\, dH(\lambda) = 0$$

The importance of the stationary reductions of the KdV hierarchy lies in the fact that (as noticed in the early works on the subject) the reduced equations can be solved by means of the classical method of separation of variables. We mention that the separability of these systems is a particular instance of a general result, which is valid for quite a wide class of bi-Hamiltonian manifolds.

Next we present an important class of bi-Hamiltonian manifolds. We recall that the dual $\mathfrak{g}^*$ of a finite-dimensional Lie algebra $\mathfrak{g}$ possesses a canonical Poisson structure, called the Lie–Poisson structure. It is defined as

$$\{F, G\}(X) = \langle X, [dF(X), dG(X)]\rangle \qquad [12]$$

where $F, G \in C^\infty(\mathfrak{g}^*)$ and their differentials at $X \in \mathfrak{g}^*$ are seen as elements of $\mathfrak{g}$. If X_0 is a fixed element in $\mathfrak{g}^*$, the constant Poisson bracket

$$\{F, G\}'(X) = \langle X_0, [dF(X), dG(X)]\rangle \qquad [13]$$

is compatible with the Lie–Poisson bracket. In fact, the Poisson pencil $\{\cdot,\cdot\}_\lambda = \{\cdot,\cdot\} - \lambda\{\cdot,\cdot\}'$ is obtained from $\{\cdot,\cdot\}$ by applying the translation $X \mapsto X + \lambda X_0$; hence, it is a Poisson bracket for every value of the constant λ. The method of translation of the argument, due to Manakov, provides a lot of bi-Hamiltonian vector fields for this bi-Hamiltonian manifold. One has to consider an Ad^*-invariant function on $\mathfrak{g}^*$, that is, a function $H \in C^\infty(\mathfrak{g}^*)$ such that

$$\langle X, [dH(X), x]\rangle = 0 \quad \forall\, x \in \mathfrak{g},\ X \in \mathfrak{g}^*$$

It is clearly a Casimir function for the Lie–Poisson bracket, and this implies that the function $X \mapsto H(X - \lambda X_0)$ is a Casimir of the Poisson pencil. If this function can be developed as a Laurent series in λ, its coefficients H_j fulfill the recursion relations

$$\{H_{j+1}, \cdot\} = \{H_j, \cdot\}' \qquad [14]$$

and thus give rise to a sequence of bi-Hamiltonian vector fields.

The last example is a generalization of the previous one. For the sake of simplicity, we consider a Lie algebra $\mathfrak{g}$ of matrices such that the trace of the product is nondegenerate, and the space $M = \mathfrak{g}^2 = \mathfrak{g} \times \mathfrak{g}$. If $F \in C^\infty(M)$, its differential at a point (x_0, x_1) can be identified with the element $(\partial F/\partial x_0, \partial F/\partial x_1)$ of M given by

$$\frac{d}{dt}_{|\epsilon=0} F(x_0 + \epsilon v_0, x_1 + \epsilon v_1) = \mathrm{tr}\left(\frac{\partial F}{\partial x_0} v_0 + \frac{\partial F}{\partial x_1} v_1\right)$$

for all $v_0, v_1 \in \mathfrak{g}$. The manifold M has a three-dimensional family of pairwise compatible Poisson brackets:

$$\{F,G\}_0(x_0,x_1) = -\mathrm{tr}\left(x_0\left[\frac{\partial F}{\partial x_1},\frac{\partial G}{\partial x_1}\right]\right)$$

$$\{F,G\}_1(x_0,x_1) = \mathrm{tr}\left(x_1\left[\frac{\partial F}{\partial x_1},\frac{\partial G}{\partial x_1}\right]\right)$$

$$\{F,G\}_2(x_0,x_1) = \mathrm{tr}\left(x_0\left[\frac{\partial F}{\partial x_0},\frac{\partial G}{\partial x_0}\right] + x_1\left(\left[\frac{\partial F}{\partial x_1},\frac{\partial G}{\partial x_0}\right] + \left[\frac{\partial F}{\partial x_0},\frac{\partial G}{\partial x_1}\right]\right)\right)$$

Notice that the first two brackets restrict to the submanifolds $x_0 = \text{constant}$ and give rise to the bi-Hamiltonian structure presented in the previous example (via the identification between $\mathfrak{g}$ and $\mathfrak{g}^*$ given by the trace of the product). This example can be generalized to an arbitrary number n of copies of $\mathfrak{g}$. In this case there is an $(n+1)$-dimensional family of pairwise compatible Poisson brackets, which can be shown to be Lie–Poisson brackets with respect to suitable Lie algebra structures on $\mathfrak{g}^n$. According to Reyman and Semenov–Tian–Shansky, these brackets can also be casted in the R-matrix formalism.

Also in this case, the Ad-invariant functions on $\mathfrak{g}$ give rise to functions in involution on our multi-Hamiltonian manifold. For example, if $H_k^{(\alpha)}$ denotes the λ^k-coefficient of $\mathrm{tr}(x_1\lambda + x_0)^\alpha$, then the recursion relations

$$\{H_k^{(\alpha)},\cdot\}_l = \{H_{k+1}^{(\alpha)},\cdot\}_{l+1}, \quad k \geq 0,\ l = 0,1$$

hold, and they imply the existence of tri-Hamiltonian vector fields on M.

Finally, we mention that the bi-Hamiltonian structure of the stationary flow of KdV – discussed above – can be obtained as a suitable reduction of the multi-Hamiltonian structure on $\mathfrak{g}^3$, where $\mathfrak{g} = \mathfrak{sl}(2,\mathbb{R})$. A similar statement holds for the other stationary flows of the Gelfand–Dickey hierarchies.

Iterative Properties and Integrability

In this section we show how to use the bi-Hamiltonian formulation of a given system to explain its integrability. In the cases similar to the open Toda lattice, where one of the Poisson structures is nondegenerate, one can introduce a recursion operator and employ its powers in order to generate a chain of integrals of motion in involution. In the other examples, where the bi-Hamiltonian structure is degenerate, the conserved quantities turn out to be the coefficients of Casimir functions of the Poisson pencil.

If $(M, \{\cdot,\cdot\}, \{\cdot,\cdot\}')$ is a bi-Hamiltonian manifold, we call bi-Hamiltonian hierarchy a sequence $\{H_k\}_{k\geq 0}$ of functions on M fulfilling the recursion relations

$$\{\cdot, H_{k+1}\} = \{\cdot, H_k\}', \quad k \geq 0 \qquad [15]$$

In terms of Poisson tensors we have that $P\,\mathrm{d}H_{k+1} = P'\,\mathrm{d}H_k$. A bi-Hamiltonian hierarchy clearly gives rise to an infinite sequence of bi-Hamiltonian vector fields,

$$X_k = P\,\mathrm{d}H_k = P'\,\mathrm{d}H_{k-1}, \quad k \geq 1 \qquad [16]$$

The functions H_k are in involution with respect to both Poisson brackets. Indeed, for $k > j$, one has

$$\{H_j, H_k\} = \{H_j, H_{k-1}\}' = \{H_{j+1}, H_{k-1}\} = \cdots = \{H_k, H_j\}$$

so that $\{H_j, H_k\} = 0$ for all $j, k \geq 0$, and therefore $\{H_j, H_k\}' = 0$ for all $j, k \geq 0$. If $\{H_i\}_{i\geq 0}$ and $\{K_i\}_{i\geq 0}$ are two bi-Hamiltonian hierarchies, then all functions are in (bi-)involution provided that one of the two hierarchies starts from a Casimir of $\{\cdot,\cdot\}$. In fact, suppose that H_0 is such a Casimir. Then

$$\{H_i, K_j\} = \{H_{i-1}, K_j\}' = \{H_{i-1}, K_{j+1}\} = \cdots = \{H_0, K_{j+i}\} = 0$$

and

$$\{H_i, K_j\}' = \{H_{i+1}, K_j\} = 0$$

We observe that these proofs of the involutivity do not use the compatibility condition [2] between the Poisson structures. The point is that this condition is important for the existence of bi-Hamiltonian hierarchies. Indeed, the problem of the existence and the construction of bi-Hamiltonian hierarchies is quite delicate. We tackle it first in the case of a particular class of bi-Hamiltonian manifolds, the so-called Poisson–Nijenhuis manifolds. In turn, they are a generalization of nondegenerate bi-Hamiltonian manifolds.

Let (M, P, P') be a bi-Hamiltonian manifold such that P is invertible. Then we can introduce the tensor field $N = P'P^{-1}$, which is of type $(1,1)$ and will always be dealt with as an endomorphism of the tangent bundle TM. This tensor field possesses some remarkable properties. First of all, its Nijenhuis torsion $T(N)$ vanishes; this means that

$$T(N)(X,Y) = [NX, NY] - N[X,Y]_N = 0$$

for any pair (X,Y) of vector fields on M, where

$$[X,Y]_N = [NX,Y] + [X,NY] - N[X,Y]$$

Sometimes a tensor field with vanishing Nijenhuis torsion is called a recursion operator. Since P defines a symplectic structure on M, such a bi-Hamiltonian manifold is called an ωN manifold.

The tensor field N satisfies two compatibility conditions with P. The first one is simply the skew-symmetry of P' and reads $NP = PN^*$, while the second one is a restatement of [3],

$$[X_F, X_G]_N = X_{\{F,G\}_{NP}} \quad \forall F, G \in C^\infty(M)$$

A manifold is said to be a Poisson–Nijenhuis manifold (briefly, a PN manifold) if it is endowed with a Poisson tensor P and a torsionless $(1,1)$ tensor field N which are compatible, in the sense that the two above-mentioned conditions hold. We have just seen that every nondegenerate bi-Hamiltonian manifold (i.e., such that one of the two Poisson tensors is invertible) is a PN manifold. On the other hand, if (M, P, N) is a PN manifold, then it can be shown that $P' = NP$ is a Poisson tensor, which is compatible with P. In other words, PN manifolds are particular examples of bi-Hamiltonian manifolds. Moreover, one has that $P^{(j)} = N^j P$ and $P^{(k)} = N^k P$ are, for every $j, k \geq 0$, compatible Poisson tensors.

Let us consider now a function H_0, on a PN manifold (M, P, N), such that $N^* \mathrm{d}H_0 = \mathrm{d}H_1$ is exact, where $N^* : T^*M \to T^*M$ is the adjoint of the recursion operator N. This implies that

$$X = P\,\mathrm{d}H_1 = PN^*\,\mathrm{d}H_0 = P'\,\mathrm{d}H_0 \qquad [17]$$

is a bi-Hamiltonian vector field. By means of N^* we can define the 1-forms $\alpha_j = (N^*)^j\,\mathrm{d}H_0$, which can be shown to be all closed. If they are exact, that is, $\alpha_k = \mathrm{d}H_k$, then the functions H_k form a bi-Hamiltonian hierarchy and thus are in involution. This shows that on a (simply connected) PN manifold every bi-Hamiltonian vector field of the form [17], with $N^*\,\mathrm{d}H_0 = \mathrm{d}H_1$, belongs to a bi-Hamiltonian hierarchy and that its first integrals (in involution) can be iteratively constructed with the recursion operator. (The integrability of this vector field clearly depends on the number of independent integrals of motion.) Moreover, the vector field $X_k = P\,\mathrm{d}H_k = P'\,\mathrm{d}H_{k-1}$ of the hierarchy is Hamiltonian with respect to all Poisson structures $P^{(j)}$ with $j \geq k$, because $X_k = P^{(j)}\,\mathrm{d}H_{k-j}$.

The example of the Toda lattice presented earlier can be casted in the PN (more precisely, ωN) framework. One can introduce the recursion operator N and, in the three-particle case, one can define the third integral of motion as $\mathrm{d}J = N^*\,\mathrm{d}H$. Since K, H, and J belong to a bi-Hamiltonian hierarchy, they are in involution, and this (along with their functional independency) proves the integrability of the Toda lattice.

In this example something more happens: the integrals of motion are (up to multiplicative constants) the traces of the powers of the recursion operator N. This is a general fact, since the vanishing of the torsion of N implies that $N^*\,\mathrm{d}I_k = \mathrm{d}I_{k+1}$, where $I_k = (1/k)\mathrm{tr}\,N^k$.

Next we deal with the case where the bi-Hamiltonian manifold (M, P, P') is not of the Poisson–Nijenhuis type, that is, both P and P' are degenerate. Let us suppose that their symplectic leaves have codimension 1. We also want to discuss in this case an iteration problem, namely the problem of constructing a bi-Hamiltonian hierarchy starting from a Casimir H_0 of P. Let us consider the Hamiltonian vector field $X_1 = P'\,\mathrm{d}H_0 = Y_{H_0}$ (using the notations introduced earlier). Thanks to the form [4] of the compatibility condition between P and P', we have that

$$L_{X_1}P = L_{Y_{H_0}}P = -L_{X_{H_0}}P' = 0$$

meaning that X_1 is an infinitesimal symmetry of P. Moreover, X_1 is tangent to the symplectic leaves of P, since $\langle \mathrm{d}H_0, X_1\rangle = \langle \mathrm{d}H_0, P'\,\mathrm{d}H_0\rangle = 0$. Under some suitable topological assumptions, we can conclude that there exists a function H_1 such that $X_1 = P\,\mathrm{d}H_1$, that is, X_1 is a bi-Hamiltonian vector field. Now the procedure can be iterated, that is, in the same way one can show that, if $X_2 = P'\,\mathrm{d}H_1 = Y_{H_1}$, then there exists a function H_2 such that $X_2 = P\,\mathrm{d}H_2$, and so on. Thus, one obtains a bi-Hamiltonian hierarchy $\{H_k\}_{k\geq 0}$, which can either be infinite or end with a Casimir of P'. In any case, the function $H(\lambda) = \sum_{k\geq 0} H_k \lambda^{-k}$ is a Casimir of the Poisson pencil $P_\lambda = P' - \lambda P$. As seen earlier, the typical situation is that the chain terminates with a Casimir H_n of P', where $\dim M = 2n+1$. In other words, there is a Casimir of the Poisson pencil which is a polynomial of degree n in the parameter λ.

As a general procedure for constructing bi-Hamiltonian hierarchies, one can look for the Casimir functions $H(\lambda)$ of the Poisson pencil which are deformations of Casimir functions of P, but it is not clear when such a deformation does exist in the case where the corank of the bi-Hamiltonian structure is greater than 2. Nevertheless, suppose that $H(\lambda) = \sum_{k\geq 0} H_k \lambda^{-k}$ is a Casimir of P_λ, that is, that $\{H_k\}_{k\geq 0}$ is a bi-Hamiltonian hierarchy. Then, for all λ, the bi-Hamiltonian vector fields $X_{k+1} = P\,\mathrm{d}H_{k+1} = P'\,\mathrm{d}H_k$ are Hamiltonian with respect to P_λ, with Hamiltonian function $H^{(k)}(\lambda) = \sum_{j=0}^{k} H_j \lambda^{k-j}$,

$$X_{k+1} = P_\lambda \mathrm{d}H^{(k)}(\lambda)$$

Therefore, the vector fields X_k are not only bi-Hamiltonian, but they are Hamiltonian with respect to any Poisson bracket of the pencil.

In this article we have described some basic properties of bi-Hamiltonian systems, defined on manifolds possessing a Poisson pair. There are other important vector fields on these manifolds (more precisely, on ωN manifolds). They are called cyclic systems of Levi-Civita, and they give an intrinsic description of the separable systems of Jacobi. We refer to the article Recursion Operators in Classical Mechanics in this encyclopedia for these topics.

See also: Bi-Hamiltonian Methods in Soliton Theory; Classical *r*-Matrices, Lie Bialgebras, and Poisson Lie Groups; Integrable Systems and Algebraic Geometry; Integrable Systems and Recursion Operators on Symplectic and Jacobi Manifolds; Integrable Systems: Overview; Recursion Operators in Classical Mechanics; Separation of Variables for Differential Equations; Solitons and Kac–Moody Lie Algebras; Toda Lattices.

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Multiscale Approaches

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Introduction: Multiple-Scale and Multiscale Approaches

Multiscale, or more precisely *multiple-scale, method* is a technique of perturbation theory based on the introduction of additional rescaled variables, say time variables, formally considered as independent variables and describing each a different timescale (for the sake of simplicity, we will mainly consider a dynamic framework and timescales; all can be transposed to spatial dependences and scales). It was first developed to handle singular situations in which dynamic regimes of different characteristic scales coexist and intermingle in such a way that straightforward perturbation expansions are not uniformly convergent in time (hence of limited relevance and use) due to the so-called *secular terms* growing unbounded with time; the freedom introduced together with the extra variables indeed allows to impose conditions preventing these secular divergences and improving the convergence of the perturbation series. It yields a global perturbation solution describing *jointly* the behavior at small and large scales. This technique belongs to the far more wide-ranging class of *multiscale approaches*; these can be divided into four main subclasses:

1. *Mean-field techniques* exploiting scale separation between fast and slow components of the dynamics. The influence of the slow variables onto the fast dynamics, if any, is treated in a decoupled way within a parametric approximation, allowing an adiabatic elimination of fast variables (see the section "Slow/fast variables").
2. *Singular perturbations*, in which individual fast components ultimately give rise to slow trends and influence the large-scale features. Scale separation here breaks down at long times and multiple-scale method is then a method of choice (see the next section).
3. *Matched expansions* when regimes of different scales succeed (boundary-layer singularity; see the section "Boundary layers and matched expansions").

4. *Renormalization techniques*, in systems exhibiting some kind of universality in the relations between their behaviors at different scales, for example, scale invariance (see the section "Renormalization: an iterated multiscale approach").

We will first present the principles of multiple-scale method, detail its technical implementation on simple abstract examples and cite some typical applications. Then we will articulate this technique with more general multiscale methods in a brief overview (see the section "A brief overview of multiscale approaches"). The range of multiscale approaches and technical tools will then be illustrated and compared in the context of diffusion, Brownian motion, and transport phenomena (see the section "Summary: the exemplary case of diffusion").

Multiple-Scale Method: Principles

Context: Singular Perturbations and Secular Divergences

Multiple-scale methods have been developed to handle situations in which the dynamics involves a small parameter ϵ (e.g., the ratio of the masses of different subsystems, the strength of an additional interaction, the amplitude of an applied field) directly controlling the separation between the different characteristic timescales of the evolution and, specifically, such that *the behavior for $\epsilon = 0$ is qualitatively different from the behavior for ϵ small* ($\epsilon \ll 1$ but finite); in other words, when a weak influence, of strength controlled by $\epsilon \ll 1$, does not have only weak consequences. Typically, this occurs when ϵ represents the strength of a weak coupling between otherwise independent subsystems or when a vanishing value $\epsilon = 0$ changes a characteristic time, the sign of a friction coefficient, the order of the highest time derivative in case of ordinary differential equations (turning points), or the type of partial differential equations in case of spatially extended systems. Accordingly, a naive perturbative approach with respect to ϵ, that is, an expansion taking as a basic approximation the behavior for $\epsilon = 0$, cannot bridge the qualitative gap with behaviors observed for $\epsilon > 0$. It thus fails to give a full account of the system evolution at all times: one speaks of *singular perturbation*.

A historical example arose in celestial mechanics, in the celebrated *nonintegrable* three-body problem, involving the Sun, a big planet and a smaller one, of respective masses $m_1, m_2 < m_1$ and $m_3 \ll m_2$. The straightforward approach would be to consider the presence of the small planet as a small perturbation of the *integrable* two-body problem for the masses m_1 and m_2. But when one tries to determine the solution as a series in powers of the mass ratio $\epsilon = m_3/m_2$, unbounded terms appear, the so-called *secular terms*, increasing without bounds as fast as t, hence of ill-defined order and impairing the very consistency of the perturbation approach at long times $t > 1/\epsilon$. Accordingly, the perturbation expansion is *not uniformly convergent in time*, preventing from using it to investigate asymptotics and determine the fate of the three-body system: the influence of the small planet on the motion of the bigger one, although seemingly a weak perturbation, might ultimately modify its trajectory around the Sun, at least in some resonant cases.

The origin of secular terms lies in a phenomenon of *resonance*, which is best explained on an example: the *Duffing oscillator* $\ddot{x} + x = -\epsilon x^3$ with $\epsilon \ll 1$. When looking for a solution in the form $x(t) = \sum \epsilon^n x_n(t)$, each component $x_n(t)$ has to be bounded in order to get a consistent perturbation expansion, in which the hierarchy of terms of different orders remains valid forever: $\epsilon x_{n+1}(t) \ll x_n(t)$. These components should satisfy the following sequence of equations:

$$\ddot{x}_0 + x_0 = 0, \quad \ddot{x}_1 + x_1 = -x_0^3, \quad \ldots \quad \text{(linearized operator } Lx \equiv \ddot{x} + x) \qquad [1]$$

It gives $x_0(t) = ae^{it} + \text{c.c.}$, from which follows a secular contribution $(3i/2)a|a|^2 t\, e^{it}$ in $x_1(t)$. In general, solving perturbatively $\dot{z} = f(z, \epsilon)$ for an expansion $z(\epsilon, t) = \sum_n \epsilon^n z_n(t)$ yields a hierarchical sequence of equations of the form $\dot{z}_n = Lz_n + \varphi_n (z_0, z_1, \ldots, z_{n-1})$ for $n \geq 1$, where $L = Df(z_0, \epsilon = 0)$ comes from the linearization in z_0 of the unperturbed evolution law. A secular divergence arises in z_n as soon as φ_n contains an additive contribution which is an eigenvector of L (part of a mathematical result known as the Fredholm alternative). The appearance of secular terms reflects a singular feature of the dynamics: the fact that the limits as $\epsilon \to 0$ and $t \to \infty$ do not commute. As a rule, such noninversion is associated with generalized secular divergences: the fast, short-term dynamics finally contributes to the slow, long-term behavior. This feature is a clue towards using multiple-scale method.

Technical Principles

The first step is to perform rescalings leading to dimensionless variables and functions, which evidence a small control parameter ϵ, related to scale separation and providing a natural parameter for a perturbation approach. The basic principle of multiple-scale method is to introduce additional *independent* time

variables $t_1, t_2, \ldots, t_n$ such that the physical situation corresponds in this extended time-variable space to the line

$$t_0 = t,\ t_1 = \epsilon t,\ t_2 = \epsilon^2 t,\ \ldots$$
$$\frac{d}{dt} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \cdots \qquad [2]$$

It thus amounts to a perturbation expansion of the time-derivative operator. This method can be traced back to the *Lindstedt–Poincaré technique*, where the time variable t is expanded according to $t = s(1 + \epsilon\omega_1 + \epsilon^2\omega_2 + \cdots)$ and the evolution described in terms of the new variable s and unknown frequencies $(\omega_i)_{i\geq 1}$ to be determined self-consistently (Nayfeh 1973). By contrast, the multiple-scale approach puts on a par $t_0 = t$ and the additional variables $(t_i)_{i\geq 1}$. The perturbation approach is then carried out as usual, plugging eqn [2] for d/dt and the expansion $z(\epsilon, t) = \sum_{n\geq 0} \epsilon^n z_n(t_0, t_1, t_2, \ldots)$ into the evolution equation and identifying term-wise the coefficients of the successive powers of ϵ. The additional freedom thus introduced when considering $(t_i)_{i\geq 0}$ as independent variables will be compensated in the course of the computation, by imposing "solubility conditions" ensuring the vanishing of secular terms and the consistency of the perturbation method. In particular, it is possible to freely choose boundary conditions outside the physical line $t_1 = \epsilon t_0, \ldots, t_n = \epsilon^n t_0$. The resulting set of equations contains exactly the same information as the original one, only expressed in a different way: by construction, terms depending, say, on t_0, describe a fast component with no emerging slow trends that would intermix with the t_1-dependence; fast variables contribute only to fast modes. At the end, one restricts to the physical line, thus turning back to the single "real" variable t. The benefit of the method is to provide a *joint access to dependences at different scales*, now expressing as dependences onto the different time variables $t_0, t_1, \ldots, t_n$. One introduces as many new variables as necessary to circumvent secular divergences. We have implicitly supposed above that the behavior at timescale $\Delta t = \mathcal{O}(1)$ corresponds to the fastest timescale of the evolution. If it were not the case, the rescaled time variables would be $t_0 = \epsilon^{n_0} t$, $t_1 = \epsilon^{n_0+1} t, \ldots$ if the fastest timescale is $\Delta t = \mathcal{O}(\epsilon^{n_0})$. More general time-derivative expansion, associated with rescaled variables $t_n = \epsilon^{\alpha_n} t$ might be considered to better account for the hierarchy of characteristic timescales of the dynamics.

Multiple-Scale Method: Abstract Examples

Let us first consider the simplest possible example $\dot{x} = a(1 + \epsilon)x$, for which the exact solution is trivially known, allowing to appreciate the validity of the multiscale approach compared to the straightforward perturbation expansion. In the latter case, one looks for a solution $x(t) = x_0(t) + \epsilon x_1(t) + \mathcal{O}(\epsilon^2)$ and identifies term-wise the powers of ϵ. At order 0, $\dot{x}_0 = ax_0$ yields $x_0(t) = c_0 e^{at}$. At order 1, $\dot{x}_1 - ax_1 = x_0(t)$ leads to a secular divergence: $x_1(t) = c_1^0 e^{at} + c_0 t e^{at}$. Carrying on the perturbation analysis yields the following expansion:

$$x(t) = c\ e^{at}(1 + \epsilon t + \epsilon^2 t^2/2 + \cdots) \qquad [3]$$

which is *not uniformly convergent*: for $t = \mathcal{O}(1/\epsilon)$, all terms are of the same magnitude. Using this recursive method to obtain a finite-order approximate solution (e.g., stopping, as here, after two steps of the perturbation method) *is only relevant at short times* $t \ll 1/\epsilon$. The straightforward perturbation analysis captures the behavior of the exact solution only if *all terms* are computed and taken into account (in less trivial examples, the straightforward perturbation series might even be divergent). In the multiple-scale approach, one introduces two rescaled variables $t_0 = t$ and $t_1 = \epsilon t$ and looks for a solution of the form $x(t) \equiv x_0(t_0, t_1, \ldots) + \epsilon x_1(t_0, t_1, \ldots) + \mathcal{O}(\epsilon^2)$. At order 0, $\partial_{t_0} x_0 = ax_0$ yields $x_0(t_0, t_1, \ldots) = c_0(t_1, \ldots)e^{at_0}$. At order 1, we get $\partial_{t_0} x_1 + \partial_{t_1} x_0 = x_0 + ax_1$. The solubility condition writes $ac_0 - \partial_{t_1} c_0 = 0$, which allows as to avoid secular divergence and suppresses the artificial freedom introduced with the additional time variable t_1, yielding $c_0 = ce^{at_1}$. The equation $(\partial_{t_0} - a)x_1 = 0$ is here superfluous, but in less simple situations, it remains at this stage a nontrivial equation for x_1. One thus directly gets the solution, uniformly valid at all times:

$$x(t) = c\ e^{at_1}\ e^{at_0} = c\ e^{a(1+\epsilon)t} \qquad [4]$$

As a rule in singular perturbation method, the difficulty here originates in the noncommuting limits $\epsilon \to 0$ and $t \to \infty$; indeed, denoting $y_\epsilon(t) = x_\epsilon(t)e^{-at}$, one has $\lim_{t\to\infty} \lim_{\epsilon\to 0^+} y_\epsilon(t) = c$, whereas $\lim_{\epsilon\to 0^+} \lim_{t\to\infty} y_\epsilon(t) = \infty$.

Other training examples are the weakly damped linear oscillator $\ddot{x} + x = -2\epsilon\dot{x}$, solved with multiple scales $t_0 = t, t_1 = \epsilon t, t_1 = \epsilon^2 t$, or with the more specific variables $\theta = \sqrt{1 - \epsilon^2}t, \tau = \epsilon t$; the Duffing oscillator $\ddot{x} + x = -\epsilon x^3$ introduced above, whose multiple-scale resolution requires three variables $t_0 = t, t_1 = \epsilon t, t_1 = \epsilon^2 t$; and the Van der Pol oscillator $\ddot{x} + x = \epsilon(1 - x^2)\dot{x}$.

An Illustration: Classical Lorentz Electron Gas in a Weak Field

As a less abstract, hence more convincing, illustration of the strength of multiple-scale method, let us

consider the dynamics of a classical Lorentz electron gas acted upon an external electric field (associated acceleration a). This model considers the electrons as charged hard spheres whose motion results from the superimposition of a driven classical motion in the field and elastic collision on immobile scatterers (the atoms). It is implemented within a kinetic-theoretic framework, based upon a Boltzmann-like equation for the electron velocity distribution:

$$\left(\frac{\partial}{\partial t} + \boldsymbol{a}.\frac{\partial}{\partial \boldsymbol{v}}\right) f(\boldsymbol{v}, t) = -\frac{v}{\lambda}\mathcal{Q}f(\boldsymbol{v}, t) \qquad [5]$$

where $v = |\boldsymbol{v}|$, and λ is the mean free path of the electrons. $\mathcal{Q}f = f - f_{\rm sph}$ is a projector accounting for the effect of collisions through the deviation of the distribution f from spherical symmetry, namely through the discrepancy between f and its isotropic counterpart $f_{\rm sph}(v) = (1/4\pi)\int f(\boldsymbol{v}, t)\mathrm{d}\hat{v}$ obtained as an average over the velocity directions $\hat{v}$. The relevant small parameter is $\epsilon = ma\lambda/kT$, measuring the ratio of the work $ma\lambda$ done by the field over the mean free path to the thermal energy kT in the initial state. The condition $\epsilon \ll 1$ ensures the separation of the characteristic timescales of the two mechanisms experienced by an electron: the thermal motion and the field-induced deterministic motion. Denoting by $v_{\rm th} = \sqrt{kT/m}$ the thermal velocity of the electrons, we have indeed $\epsilon = (t_{\rm th}/t_{\rm acc})^2$, where $t_{\rm th} = \lambda v_{\rm th}$ is the mean time between two successive collisions with the scatterers and $t_{\rm acc} = \sqrt{\lambda/a}$ is the acceleration time required for the field to move the electron over the mean free path λ starting from rest. The result of the plain weak-field expansion is to evidence its own failure: it shows that the perturbation is singular insofar as the asymptotic state will be fully dominated by the field, with no memory of the initial temperature. Multiple-scale method is here implemented with respect to the time variable, introducing new independent variables $(\tau_i)_{i>0}$ such that the physical situation corresponds to the line

$$\tau_0 = tv_{\rm th}/\lambda,\ \tau_1 = \epsilon\tau_0,\ \tau_2 = \epsilon^2\tau_0,\ \ldots,\ \tau_n = \epsilon^n\tau_0,\ \ldots \quad (\epsilon = ma\lambda/kT) \qquad [6]$$

The time-derivative expansion [2] is supplemented with an expansion of the velocity distribution:

$$f(\boldsymbol{v}, t) = \sum_{i\geq 0} \epsilon^i F^{(i)}(\boldsymbol{v}, \tau_0, \tau_1, \ldots, \tau_n, \ldots) \qquad [7]$$

The procedure is conducted as exposed in the general case. Identifying term-wise the coefficients of the expansion yields a hierarchy of equations for the $(F^{(i)})_{i\geq 1}$, each supplemented with a solubility condition preventing the appearance of secular divergences. A detailed presentation can be found in Piasecki (1993). The benefit of the multiple-scale method is to yield *jointly* the different stages of the gas evolution, starting from thermal equilibrium and switching on the field at $t = 0$:

- at times $\tau = \mathcal{O}(1)$, an initial transient with a drift velocity $\langle v_z\rangle(t) = at - C_1 at^2 v_{\rm th}/\lambda + \cdots$ in the direction of the applied field (denoting C_1 some numerical constant);
- at times $\tau = \mathcal{O}(1/\epsilon)$, a linear-response regime with a steady drift velocity $\langle v_z\rangle \sim a\lambda/v_{\rm th}$; and
- at times $\tau = \mathcal{O}(1/\epsilon^2)$, a long-time field-dominated heating of the gas, where the velocity distribution is no longer Maxwellian, and the kinetic energy of the electrons grows without bounds as $t^{2/3}$, whereas the drift velocity slowly vanishes asymptotically: $\langle v_z\rangle \sim (\lambda^2 a/t)^{1/3}$.

Domains of Application of the Multiple-Scale Method

The multiple-scale method was first developed in nonlinear mechanics. It is fruitful and is even required in any instance where plain perturbation expansion is not uniformly convergent, more generally when it is necessary to account jointly for variations at different timescales: resonant wave interactions, for example, in plasmas, or in the case of oscillations with slowly varying coefficients. Multiple-timescale method was applied, around 1960, to get kinetic equations (closed equations for the one-particle distribution) from molecular dynamics (Liouville equation) for dilute gases, plasmas, or to establish a microscopic theory of Brownian motion from molecular dynamics of a hard-sphere system (see the section "Microscopic theory of Brownian motion"). In the same spirit, it allows to relate constructively different mesoscopic descriptions, for example, in the case of Brownian motion, to relate the Kramers equation for the distribution $P(\boldsymbol{r}, \boldsymbol{v}, t)$ to the Smoluchowski equation for $P(\boldsymbol{r}, t)$ (see the section "Mesoscopic theory of Brownian motion"). Other examples are the determination of transport coefficients (friction, viscosity) from kinetic description or, at macroscopic scale, the determination of eddy viscosity and eddy diffusivity (see the section "Effective diffusivity for a passively advected scalar"). A last domain of application concerns systems where relaxation processes at different scales superimpose, requiring to handle jointly different time dependences. Multiple-scale method then displays the physics of the relaxation process and its associated hierarchical structure (e.g., the application to the adiabatic piston problem discussed in this Encyclopedia by

Gruber and Lesne – *see* Adiabatic Piston; see also the section "Some typical applications").

A Brief Overview of Multiscale Approaches

Different Scales and Regimes

Common to all multiscale approaches is the *focus on the very existence of different scales*, exploited through the use of rescaled variables, which makes explicit the presence of a small parameter ϵ controlling the dynamics, responsible for the existence of different timescales and related to the scale separation. Technically, the first, very simple but essential, step is to replace the variables, fields, and parameters by their dimensionless counterparts. So doing, small parameters reflecting scale separation (in time, space, energies, amplitudes,...) will naturally appear. Although it is thus possible to estimate the order of the different terms, it is to be underlined that *it gives no clue on their actual contribution to the long-term behavior*: in singular situations, precisely those where multiscale approaches have to be developed, small terms can have a noticeable influence at all scales. As illustrated in the following sections, different rescalings of variables and functions allow us to discriminate features at different scales and to capture different regimes. More specifically, the techniques to manage with the joint contributions of several regimes at different timescales depend on the way these regimes intermix. They can be:

- *superimposed* regimes, when fast and slow dependences intermingle in the evolution of the same variable. It is the framework of multiple-scale analysis. The solution writes typically $x(t, \epsilon t, \epsilon^2 t, \ldots)$; or
- *coexisting* regimes, namely a coexistence of fast and slow evolutions. One might focus either on the fast evolution and use a quasistatic approximation (or parametric approximation) for the slow evolution, either on the slow evolution and use a quasistationary approximation or an averaging of the fast evolution. The solution writes typically $[x_{\text{fast}}(t), x_{\text{slow}}(\epsilon t)]$ (or $[x_{\text{fast}}(\tau/\epsilon), x_{\text{slow}}(\tau)]$ if the observation takes place at long timescales, with a relevant time variable $\tau = \epsilon t$); or
- *successive* regimes, when initial conditions, bulk behavior and asymptotics are not of the same order with respect to ϵ; this is a boundary-layer-like issue, and the solution writes typically $x_{\text{layer}}(t/\epsilon)$ for $0 \leq t \leq t_0$, then $x_{\text{bulk}}(t)$ for $t \geq t_0$, with $t_0 = \mathcal{O}(1)$.

Applications are innumerable; the most typical and investigated ones are the climate (from "hours" for the observed weather to "thousands of years" for eras), population dynamics, coasts and sand dunes (from "grains" to "country" scales), protein folding (the vibration of covalent bonds occurs at scale of femtoseconds, while the whole folding may require up to a few seconds), or trading markets (from seconds to years). Let us finally give two typical examples for the parameter ϵ:

- *The weak-damping and high-friction limits*, best explained on an example. The damped oscillator $m\ddot{x} + \gamma\dot{x} + V'(x) = 0$ appears as an *Hamiltonian dynamics* $m\ddot{x} + V'(x) = 0$ as soon as the damping can be neglected, when the characteristic time $\theta = [m/V''(0)]^{1/2}$ of the undamped oscillator is far smaller than the damping time $\tau = m/\gamma$. The weak-damping limit is thus defined as $\epsilon \to 0$, where $\epsilon = \theta/\tau = [\gamma^2/mV''(0)]^{1/2}$. It leads to a singular behavior when investigating the asymptotics, as in the Duffing oscillator and weakly damped oscillator mentioned in the last section. On the contrary, the evolution appears as a *dissipative gradient dynamics* $\dot{x} = -V'(x)/\gamma = 0$ as soon as $\tau \ll \theta$. This leads to the high-friction limit: $\tau/\theta = [mV''(0)/\gamma^2]^{1/2} \to 0$. This example somehow reconciles conservative and dissipative dynamics, showing that they might coexist in the same system.
- *The hydrodynamic limit* involved in the derivation of hydrodynamics equations (namely incompressible Navier–Stokes equations) from kinetic Boltzmann equation. It writes $\epsilon = \lambda/L \to 0$, where ϵ is the so-called *Knudsen number*, defined as the ratio of the mean free path λ (the average distance traveled by a fluid molecule between two successive collisions) to a characteristic spatial scale L of the system (e.g., the size of an obstacle).

Bridging the Scales: Mean-Field, Singular and Scaling Approaches

The aim of multiscale approaches is to bridge different scales, through the determination of the large-scale behavior of the solution, or by establishing a constructive relation between the initial model and an effective model at higher scale. We have mentioned in the introduction a first classification of multiscale systems and associated approaches: they might exhibit (1) scale decoupling, (2) some singularity in the relation between the different scales, or (3) scale invariance.

Mean-field approaches In case of scale decoupling, mean-field approaches apply. Let us briefly recall,

within its usual spatial formulation, that a mean-field approach amounts to identifying the local environment, which is *a priori* fluctuating and spatially inhomogeneous (e.g., the local magnetic field generated by neighboring spins in a spin lattice model) with the average one, expressed as a function of the average order parameter (spatial average or equivalently a statistical average in the limit as the system size tends to infinity). Mean-field approaches can be implemented either in time (*averaging*), in real space (*homogenization*, *coarse-graining*), or in phase space (*aggregation and projection techniques*).

In the present context, the best example of a mean-field approach is provided by *homogenization* procedures. They can be traced back to the method of Lagrange to solve the three-body problem. The issue is to describe the motion of a light body B_2 experiencing the gravitational attraction of the Sun and a heavier body B_1. The mass of B_2 is supposed to be small enough to neglect its influence on the Sun and B_1 (the so-called restricted three-body problem); B_1 will thus obey the Keplerian laws of motion. The method of Lagrange applies when B_2 is far more distant from the Sun than $B_1 (r_2 \gg r_1)$, which implies (due to the third law of Kepler: $\omega^2 r^3 = \text{const.}$) that the angular velocity ω_1 of B_1 is far larger than ω_2: the large body B_1 moves faster than B_2 around the Sun. In first approximation, Lagrange replaced the rapidly oscillating influence of B_1 on the motion of B_2 by the influence of a constant distribution of mass, obtained by spreading the mass m_1 of B_1 all over its orbit. The Gauss theorem thus states that this influence can be accounted for by simply adding the total mass of this distribution to the mass of the Sun. The stability of the system would follow: B_2 will remain trapped in the neighborhood of the pair composed with the Sun and B_1.

Singular perturbations A typical instance of singular multiscale behavior is associated with asymptotic expansions

$$x(t) = \sum_{r=0}^{n-1} \epsilon^r x_r + R_n(\epsilon, t) \qquad [8]$$

which are *not* convergent: $\lim_{n\to\infty} R_n(\epsilon, t) \neq 0$ at ϵ fixed, but $\lim_{\epsilon\to 0} \epsilon^{-n} R_n(\epsilon, t) = 0$ at fixed n and t. Asymptotic expansions are ubiquitous in multiscale approaches: the coexistence of different timescales, superimposed and nontrivially coupled to get rise to the observed phenomenon, prevents from obtaining uniformly convergent perturbative expansions; it is only in this latter regular case that the above-mentioned mean-field approaches and homogenization techniques apply.

Scale invariance, scaling theories and renormalization Self-similarity and associated criticality prevent scale decoupling, but allow us to develop scaling theories and renormalization methods. In contrast to scale-separation arguments, the guiding principle is now to focus on the links relating one scale to the others (scaling transformations, renormalization transformations). The problem complexity is thus reduced in a some "transverse way," by retaining only scale-invariant features. We shall expose in the section "Renormalization: an iterated multiscale approach" further links between multiscale approaches and renormalization methods, beyond the restricted scope of scale-invariant systems: in many instances, renormalization can be seen as an iterated multiscale approach.

Scaling Limits

Let us mention a specific instance of multiscale approach, which is associated with scaling limits. Scaling limit refers to a joint limiting procedure, in which several independent variables *jointly* converge towards given limits, with *prescribed relative behaviors*; this latter condition is a key point in the frequent case when the different limits do not commute, and we shall see later that it is an essential ingredient of renormalization methods. Let us cite two acknowledged examples:

- *The thermodynamic limit* for a system of N particles in a volume V; it amounts to let $N \to \infty$, $V \to \infty$, while $N/V = n = \text{const.}$ (constant average number density). It is a prerequisite to derive standard thermodynamic behavior from the statistical–mechanical description; it supports the use of asymptotic results given by the law of large numbers and the central-limit theorem provided the correlations between the particles remain short-range.
- *The Boltzmann–Grad limit* for a system of n hard spheres of radius ϵ per unit volume. In dimension d, it writes $\epsilon \to 0, n \to \infty$ (thus differing from the thermodynamic limit) while $n\epsilon^{d-1} = z$ remains constant. This limit is involved in kinetic theory as a limiting instance where the Boltzmann ansatz applies (identifying the two-particle distribution function with the product of the corresponding one-particle distributions). Indeed, the occupied volume fraction $n\epsilon^d$ tends to 0 so that recollisions and ensuing long-term correlations can be neglected (rarefied gas). On the other hand, the mean free path of a particle remains finite, so that numerous collisions and associated molecular chaos further support the Boltzmann decorrelation ansatz.

Stochastic Multiscale Approaches

Multiscale approaches are far less developed for stochastic processes. Let us mention the case of a Markov process. Scale separation reflects in a spectral gap in the transition matrix generating the dynamics. Identification of fast and slow modes is then straightforward: slow modes are associated with quasidegenerated eigenvalues ($\lambda \approx 0$ in a time-continuous setting), whereas fast dynamics is associated with damped modes and negative eigenvalues ($\lambda < 0, |\lambda| \gg 1$) (Gaveau *et al.* 1999). A basic difficulty in extending methods developed in a deterministic context is the fact that the reduction (or projection) of a Markov process is *a priori* no longer Markovian. Closure relations and approximations should be introduced to circumvent memory effects, for example, supported by arguments of decorrelation and ensuing fast temporal self-averaging of the fast dynamics.

It is to note that the behavior upon rescaling of a stochastic process differs from the transformation of a deterministic evolution. The basic relation is the scaling upon a time rescaling $\theta = \epsilon t$ of the white noise involved in stochastic differential equations and defined from the Wiener process $W(t)$ through the relation $\mathrm{d}W(t) = \eta(t)\mathrm{d}t$. It follows from the definition $\widetilde{W}(\theta) = W(t)$ that $\mathrm{d}\widetilde{W}(\theta) = \sqrt{\epsilon}\,\mathrm{d}W(t)$. At this point, it is important to notice the difference with respect to the behavior of a plain deterministic function $\tilde{f}(\theta) = f(t)$ for which $\mathrm{d}\tilde{f}(\theta) = \epsilon\,\mathrm{d}f(t)$. Using the fact that $\delta(t) = \epsilon\delta(\theta)$ and the definition $\mathrm{d}\widetilde{W}(\theta) = \tilde{\eta}(\theta)\mathrm{d}\theta$, we obtain that $\tilde{\eta}(\theta)$ is a white noise with respect to the rescaled time θ, that is, a stationary Gaussian process defined by its first two moments

$$\langle \tilde{\eta}(\theta) \rangle = 0, \qquad \langle \tilde{\eta}(\theta)\tilde{\eta}(\theta') \rangle = \delta(\theta - \theta') \qquad [9]$$

Slow/Fast Variables

Slow/Fast Decomposition

Dynamics of systems made of many interacting elements, for example, chemical reactions, or population dynamics, typically involves far too many degrees of freedom to be handled at the level of individual units, and requires a drastic reduction to make sense of it. A natural way of reduction is based upon the phenomenology, taking as relevant degrees of freedom those describing the slow evolution observed at macroscopic scales. Scale separation between microscopic and macroscopic worlds has to be turned into a constructive and quantitative argument to achieve this reduction.

Solving this typical multiscale issue first requires *to identify and construct explicitly the slow variables*, for example, collective variables obtained through aggregation or coarse-grainings. The second step is *to eliminate or rather integrate the fast dynamics* into a closed system of effective equations describing the large-scale evolution. The closure requirement generically involves an approximation, neglecting the remaining dynamic coupling between fast and slow variables. It is precisely here that scale-separation arguments and the very choice of the slow variables are crucial, ensuring that the influence of fast dynamics is essentially accounted for in its effective or average contribution to the slow dynamics; remaining fluctuating influences can be either neglected or included in a noise term, required to be fully determined as a function of the slow variable only (otherwise the whole procedure would neither be consistent nor useful). In the following subsections, we shall briefly present the main techniques allowing to achieve this program, considering the simple abstract system:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = f(X, Y), \frac{\mathrm{d}Y}{\mathrm{d}t} = \epsilon g(X, Y), \quad (\epsilon \ll 1) \qquad [10]$$

Although involving only two variables for simplicity, it exhibits the typical multiscale structure: whereas X varies on scales $\mathcal{O}(1)$, Y appears as a slow variable of characteristic timescale $\mathcal{O}(1/\epsilon)$.

Parametric Approximation

The preliminary step of the reduction is to get some knowledge on the fast dynamics, at least to choose the proper multiscale technique. A plain but nevertheless fruitful remark is that a parameter p can always be seen as a variable that does not evolve: $\mathrm{d}p/\mathrm{d}t = 0$ in a deterministic setting, or $W_{p \to q} = \delta(p - q)$ in a stochastic one (transition probability W). Conversely, a slow variable can be transiently treated as a mere parameter in the fast dynamics. Supported by timescale separation, this *parametric approximation* (or *quasistatic* approximation) decouples the fast dynamics from the slow variable evolution, investigating the fast dynamics asymptotics ($t \to \infty$) while considering that the slow variable remains constant $Y(t) \equiv y$. In the following, we shall distinguish two cases: (1) the fast dynamics oscillates with a period $T \ll 1/\epsilon$, and (2) the fast dynamics relaxes to a stable equilibrium point $X^*(y)$ slaved to the slow variable.

Amplitude Equations

A ubiquitous technique to account for *slowly modulated oscillations* has been introduced first by

Fresnel for light propagation and optical phenomena. The basic idea is to take benefit from the scale separation between the fundamental oscillation (frequency ω, wavelength $\lambda = 2\pi/k$) and a superimposed slow variation of the wave amplitude

$$\mathcal{A}(\boldsymbol{r}, t) = A(\boldsymbol{r}, t)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}.\boldsymbol{r}-\omega t)} \qquad K \equiv |\nabla A/A| \ll k, \qquad \Omega \equiv |\partial_t A/A| \ll \omega \qquad [11]$$

The evolution can be rewritten in terms of the slowly varying amplitude A; by construction, it is ruled by terms involving the small parameter $\epsilon \sim K/k \sim \Omega/\omega \ll 1$, but the resulting equation is now devoid of small or large parameter. Such technique has been successfully applied and further developed, for example, in various situations involving *electromagnetic waves* (e.g., diffraction of Hertzian waves), in *plasma physics* (resonant interaction between electromagnetic waves and acoustic modes) and in *quantum mechanics*, to investigate the deformation of a wave packet in a potential.

Averaging

Let us discuss further, in a general setting, the case when the fast dynamics is an oscillation of period T (either linear modes as in the last subsection or a stable limit cycle). It is a context where *averaging techniques* apply. We refer to the associated entry in this Encyclopedia by Neishtatdt (see the article Averaging Methods) and only mention here the main principle: to exploit scale separation and self-averaging property of the fast dynamics to replace $X(t)$ by an average value

$$X_{\mathrm{av}}(t) = (1/T)\int_t^{T+t} X(s)\mathrm{d}s$$

The underlying idea is that averaging cancels out most of the fast variations so that $X_{\mathrm{av}}(t)$ is now slowly varying. In case when the fast dynamics is influenced by the slow variable Y, its value is kept constant in the averaging (see the section "Parametric approximation"). The resulting average behavior $X_{\mathrm{av}}[Y(t), t]$ is reinjected in the evolution of the slow component, leading to a closed equation,

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = \epsilon\, g(X_{\mathrm{av}}[Y(t), t], Y)$$

or rather [12]

$$\frac{\mathrm{d}\tilde{Y}}{\mathrm{d}\tau} = g\left(\tilde{X}_{\mathrm{av}}[\tilde{Y}(\tau), \tau], \tilde{Y}\right)$$

in terms of the more relevant rescaled time variable $\tau = \epsilon t$ and $\tilde{Y}(\tau) \equiv Y(t)$. Denoting $\bar{Y}(\tau)$ the solution of this approximate equation, the validity of the averaging procedure is assessed by theorems giving conditions ensuring that $\lim_{\epsilon\to 0} \tilde{Y}_\epsilon(\tau) = \bar{Y}(\tau)$. Note that such theorems (quite unusually) state the convergence, for a vanishing value of the perturbation parameter ϵ, of the exact solutions towards the approximate one (solution of the average equations).

To conclude, let us notice that one speaks of averaging in temporal context and homogenization in spatial or spatio-temporal contexts, when averaging is performed over space; as discussed in the section "Bridging the scales: mean-field, scalar, and scaling approaches," averaging and homogenization belongs to the general class of mean-field approximations.

Quasistationary Approximation

Let us now consider the case when the fast dynamics converges at fixed Y towards a stable fixed point $X^*(Y)$. Focusing on the slow dynamics, the relevant time variable is $\tau = \epsilon t$, which turns the evolution [10] into

$$\epsilon\frac{\mathrm{d}X}{\mathrm{d}t} = f(X, Y), \qquad \frac{\mathrm{d}Y}{\mathrm{d}t} = g(X, Y) \qquad [13]$$

(for the sake of simplicity, we use the same notation X for both $X(t)$ and $\tilde{X}(\tau)$). It is solved in two steps, by noticing that at lowest order in ϵ, the fast dynamics reduces to the asymptotic regime $f(X, Y) = 0$, slaved to the slow variable Y. The corresponding stable state $X^*(Y)$ is then plugged into the slow dynamics to get a closed equation for $Y(\tau)$:

$$\frac{\mathrm{d}Y}{\mathrm{d}\tau} = g[X^*(Y), Y] \equiv G(Y) \qquad [14]$$

This achieves the desired dimensional reduction. It works equally well when X is a string of variables $X = (x_1, \ldots, x_N)$.

There is seemingly a paradox here, ubiquitous in many multiscale approaches: in order to determine the evolution of the slow variable Y, it is considered a constant! The solution lies in scale separation: the trick is to consider the ensuing approximate decoupling as an exact one (what it would be in the limit $\epsilon \to 0$). In other words, the constancy of Y is considered over a time length which is long at the level of fast dynamics ($\Delta t \gg 1$), long enough for X to reach its equilibrium state $X^*(Y)$, but short at the macroscopic level ($\epsilon\Delta t = \Delta\tau \ll 1$). As in the so-called "quasistatic evolutions" encountered in thermodynamics, the large-scale evolution will be composed of a continued succession of local equilibrium states: at each time τ, X takes its instantaneous equilibrium value, slaved to $Y(\tau)$. Here one speaks equivalently of *quasistationary*

approximation, *quasisteady-state approximation*, or *adiabatic elimination of fast variables*.

Slow Invariant Manifolds

In the previous subsections, the decomposition between fast variables X and slow variables Y was given. But in practice, only the whole dynamics of the system is known and a main part of the issue is to find and construct explicitly the slow variables.

A geometrical viewpoint on the dynamics appears to be fruitful: if the system evolution is to be reducible to the evolution of a few degrees of freedom, it means that the flow essentially lives in a low-dimensional region of the phase space, which can be parametrized by these degrees of freedom up to some fuzziness of order $\mathcal{O}(\epsilon)$. Mathematical investigations have been conducted to assess this point, leading to the concept of *invariant slow manifold*: a manifold $\mathcal{M}$ of the phase space, invariant upon the dynamics and describing the slow dynamics once the system has reached it (Gorban *et al.* 2004). Starting from an arbitrary point z_0, the trajectory first exhibits a fast transient bringing the system state close to $\mathcal{M}$, up to some tolerance of order $\mathcal{O}(\epsilon)$, then sticks to $\mathcal{M}$. Its evolution on $\mathcal{M}$ is ruled by a reduced dynamics, far slower than the fast relaxation to $\mathcal{M}$ as soon as the system actually exhibits a timescale separation. This latter self-consistent assertion should be considered as a working hypothesis, to be validated by the explicit determination of $\mathcal{M}$ and associated reduced dynamics. This can be done numerically, by exploiting the presumed convergence property of any trajectory reaching $\mathcal{M}$ after some intrinsic transients. In other words, if the dynamics possesses a slow invariant manifold, an operational way to find $\mathcal{M}$ is to let the system evolve, starting from a sample of initial conditions, and to observe its stabilization on $\mathcal{M}$.

This framework obviously embeds the quasistationary approximation presented in the last subsection: in this case, the slow invariant manifold is $\mathcal{M}=\{z=(x,y), f(z)=0\}=\{(x^*(y),y)\}$ and the dynamics restricted to $\mathcal{M}$ is the slow dynamics $dy/d\tau = G[y(\tau)]$, $x(\tau)=x^*[y(\tau)]$. Here the manifold is invariant upon the approximate dynamics (for all t, $f[z(t)]=0$, hence $z(t)\in\mathcal{M}$) but not upon the original one: some rigorous mathematical work has to be done to show that the actual dynamics keeps the trajectory in a proper neighborhood of $\mathcal{M}$ of width $\mathcal{O}(\epsilon)$. In other words, one has to control the discrepancy between the exact trajectory and the trajectory slaved on $\mathcal{M}$.

Central Manifold

The notion of slow invariant manifold generalizes older results about *central manifolds*, exploited to reduce the dynamics *near a bifurcation point*. Let us consider a dynamical system $\dot{x}=f(x,\alpha)$ near a bifurcation point: in $\alpha=\alpha_c$, the fixed point x_0, stable for $\alpha<\alpha_c$, loses its stability. This reflects on the largest eigenvalue(s) of the stability matrix $Df(x_0,\alpha)$, namely $\lambda_1(\alpha)<0$ for $\alpha<\alpha_c, \lambda_1(\alpha)>0$ for $\alpha>\alpha_c$, and $\lambda_1(\alpha_c)=0$. The small parameter is then $\epsilon=\lambda_1$. A main result was to show that, near the bifurcation point, slow modes coincide with unstable directions and fast modes with stable directions (Haken 1996). The decomposition into slow and fast variables is ruled by the *central manifold theorem*: the solutions can be expressed in terms of the amplitudes along the eigenvectors of the null space of the dynamics at $\epsilon=0$; these amplitudes appear as the relevant *order parameters* near the bifurcation. This is referred to as the *slaving principle*. Compared to the setting presented in the subsection "Slow invariant manifolds," the slow invariant manifold $\mathcal{M}$ is given here by the central manifold.

Projection Techniques

The methods presented in the previous subsections to eliminate fast variables and construct a reduced slow dynamics can be unified into a common framework: *Mori–Zwanzig projection techniques*. The full state (x, y) of the system is projected onto the slow variable y and the functions $w(x, y)$ are projected onto their conditional expectation

$$\mathcal{P}w(y) \equiv \int w(x,y)\rho(x|y)\mathrm{d}x \qquad [15]$$

The core of the method lies in the choice of conditional distribution $\rho(x\,|\,y)$, for instance, $\rho(x\,|\,y)=\delta(x-x^*(y))$ in case when there is an invariant manifold $x=x^*(y)$, or $\rho(x\,|\,y)=1/2\pi$ in case of averaging over a rapidly varying phase x. We refer to Givon *et al.* (2004) for a review.

Aggregation Techniques and Coarse-Grainings

An intuitive guideline in the analysis of a multiscale dynamics is that *collective variables or coherent states coincide with slow modes*. The rationale is that numerous fast fluctuations at the level of agent dynamics self-average, so that only a slow trend is perceptible at large scale. *Aggregation methods* have been developed in this spirit to build reduced models governing the slow dynamics. Nevertheless, in generic situations, aggregation does not lead to

closed equations for the collective variables and some level of approximation has to be introduced.

Let us now consider a system of N coupled degrees of freedom, $[x_i(t)]_{I=1...N}$ (e.g., a system of N interacting agents) evolving deterministically according to a two-scale dynamics (Auger and Bravo de la Parra 2000):

$$\epsilon \frac{dx_i}{dt} = f_i(x_1, \ldots, x_n) + \epsilon g_i(x_1, \ldots, x_n) \qquad [16]$$

where f describes a fast evolution due to the coupling between species and g_i a slow evolution due to internal mechanisms. A natural choice for the slow variable is $Y(x_1, \ldots, x_n) = \sum_i x_i$, but we shall write below the general case. The self-consistent requirement of the method is that this variable Y reflect a global and slow behavior. Considering t as a fast time variable, this condition amounts to require a quasistatic behavior for Y at this timescale. In other words, the consistency condition requires that there exists a manifold $\mathcal{F}_y$ such that

$$\sum_{i=1}^{N} \frac{\partial Y}{\partial x_i}(x_1, \ldots, x_N) f_i(x_1, \ldots, x_N) = 0$$
$$\text{on } \mathcal{F}_y = \{Y(x_1, \ldots, x_N) = y\} \qquad [17]$$

We, moreover, assume that the fast dynamics on this manifold $\mathcal{F}_y$ leads to a stable equilibrium $(x_1^*(y), \ldots, x_N^*(y))$. We are then in a position to describe the slow evolution of the manifold itself, that is, the slow dynamics ruling the evolution of the aggregated variable y for ϵ small enough:

$$\frac{dy}{dt} = \sum_i \frac{\partial Y}{\partial x_i}[x_1^*(y), \ldots, x_N^*(y)]$$
$$\times g_i[x_1^*(y), \ldots, x_N^*(y)] + \mathcal{O}(\epsilon) \qquad [18]$$

Internal support of the procedure is to check the structural stability of this resulting aggregated dynamics. Compared to the quasistationary approximation and slaving principle presented earlier, here the slow variable is not given independently but constructed as a function of the fast variables (aggregated variable). The same principles can also be implemented for discrete-time models.

Coarse-graining can be seen as the spatial analog of aggregation techniques developed in the phase space: the real space is split into cells considered as elementary units at macroscopic scale, and all the small-scale physics is averaged over each cell, yielding the apparent state of each unit (described by a few "coarse-grained" variables) and the effective interactions between them.

Let us cite two hydrodynamic examples. *Eddy viscosity* refers to an effective viscosity involved in coarse-grained hydrodynamics equations; the contribution of small-scale turbulent structures is accounted for in an integrated way in this parameter, hence its name. It is typically lower than bare viscosity, even possibly reaching negative values at large enough Reynolds number, that is, at low enough bare viscosities. *Cellular flows* are space-periodic flows, thus exhibiting a natural spatial scale: the coarse-graining amounts to an intrinsic homogenization over each cell of the flow.

Let us finally mention that coarse-grainings are involved in renormalization-group transformations once supplemented with the adequate rescalings (see the section "Renormalization: an iterated multiscale approach").

In conclusion, it is to note that all these various multiscale approaches are closely related and can all be expressed as a specific projection technique in the extended phase space containing both fast and slow variables. For instance, aggregation techniques replacing the fast variables $(x_1, \ldots, x_n)$ by the slow collective variable $y = Y(x_1, \ldots, x_n)$ amount to the projection technique involving the slow invariant manifold $\mathcal{M} = \{(x_1, \ldots, x_n, y) \mid y = Y(x_1, \ldots, x_n)\}$.

Numerical Aspects

In the community of applied mathematics, multiscale methods refer specifically to numerical homogenization, involving *multigrid algorithms* as, for instance, multiscale finite-element method, multigrid Monte Carlo, multigrid optimization, or annealing. Basically, the idea of numerical homogenization is to avoid the numerical cost of using a mesh of size $h < \epsilon$, where ϵ is the scale of the smallest-scale features of the dynamics, and to use jointly:

- a fine mesh, to compute local quantities independently (hence with a parallelized program); and
- a coarse mesh, to compute global behavior using effective parameters and homogenized quantities determined in the prior fine-mesh computation.

We refer to Gorban *et al.* (2004) for a review.

Boundary Layers and Matched Expansions

Purposes and Principles

Multiscale approach to handle boundary layers was introduced in 1905 by Prandtl in fluid mechanics for situations where the solution of hydrodynamics equations far from the boundaries ("bulk" solution) does not match the conditions at the surface of the walls or obstacles. This typically originates in the presence of a multiplicative small factor ϵ in front of

the highest-order derivative; accordingly, the flow exhibits two different scales in space: a thin boundary layer of width controlled by ϵ and the bulk domain. The idea is to perform two different perturbation methods in the layer and in the bulk, involving a different rescaling in order to focus on and give the ruling place to either the boundary conditions or the bulk dynamics (one also speaks of *inner* and *outer* expansions). Then these parallel perturbation expansions have to be bridged into a single global continuous solution. The matching principle is to identify the asymptotic behavior on the boundary side with the boundary condition of the bulk behavior (Nayfeh 1973):

$$\lim_{r\to 0} X_{\text{bulk}}(r) = \lim_{\zeta\to\infty} X_{\text{layer}}(\zeta) \quad \text{with } \zeta = r/\epsilon \qquad [19]$$

Boundary layers of hydrodynamics have numerous analogs: *initial layers* in chemical kinetics, *skin layers* in electrodynamics and *edge layers* in solid-state physics (Nayfeh 1973). Adaptation of this technique is to be developed to determine the complete dynamics in the slow-invariant-manifold approach, matching the fast relaxation towards the manifold with the slow motion onto the manifold. Let us finally note that the matched-expansion approach can benefit in each region of all the above-mentioned multiscale techniques.

Time Analog: Implementation for Initial Layers

We shall now work out the time analog of a boundary-layer problem on the abstract example encountered in [10], in the case when X rapidly evolves to a slaved equilibrium state $X^*(Y)$ but with initial conditions $Y(0)=y_0$ and $X(0)=x_0 \neq X^*(y_0)$. Obviously, the quasistationary approximation fails to describe the initial regime and its applicability has to be reconsidered. The general principle of boundary-layer analysis, namely the recourse to two different perturbation approaches, is implemented as follows:

- For the initial regime, one solves the fast dynamics with initial conditions $X(0)=x_0$ while keeping $Y(t)\equiv y_0$; this yields an approximate solution $[X_{\text{layer}}(t), Y_{\text{layer}}(t)]$, satisfying the initial conditions and valid at short times, as long as Y has not evolved.
- At longer times, the relevant variable is the rescaled time $\tau=\epsilon t$ and the quasistationary approximation described in the last section applies.

The consistency of the two perturbative approaches is ensured by the *matching conditions*

$$\begin{aligned} \lim_{\tau\to 0} X_{\text{bulk}}(\tau) &= \lim_{t\to\infty} X_{\text{layer}}(t) \\ \lim_{\tau\to 0} Y_{\text{bulk}}(\tau) &= \lim_{t\to\infty} Y_{\text{layer}}(t) \equiv y_0 \end{aligned} \qquad [20]$$

These conditions are actually satisfied since $X_{\text{bulk}}(\tau) \equiv X^*[Y_{\text{bulk}}(\tau)]$, hence $\lim_{\tau\to 0} X_{\text{bulk}}(\tau)=X^*(y_0)$ and, by definition of X^* (at fixed $Y(t)\equiv y_0$), $\lim_{t\to\infty} X_{\text{layer}}(t)=X^*(y_0)$.

Some Typical Applications

Enzymatic catalysis A matched singular perturbation approach is currently encountered in chemical systems, for instance, in the derivation of the *Michaelis–Menten kinetics* for a single enzyme and the *Hille cooperative kinetics* for an allosteric enzyme (Murray 2002). Denoting by E the enzyme, by S the substrate, by ES the active complex, and by P the product, the single-enzyme catalytic transformation of S into P is described by the following scheme:

$$\begin{aligned} &S + E \underset{k'}{\overset{k}{\rightleftharpoons}} ES \xrightarrow{k_{\text{cal}}} P + E \\ &[S]\equiv s, \quad [E]\equiv e, \quad [ES]\equiv c \end{aligned} \qquad [21]$$

where, as is well known, the enzyme is released at the end. Introducing dimensionless quantities

$$\begin{aligned} &\tilde{t} \equiv ke_0 t, \quad \tilde{s} \equiv \frac{s}{s_0}, \quad \tilde{c} \equiv \frac{c}{e_0} \\ &K_{\text{m}} \equiv \frac{k' + k_{\text{cat}}}{k}, \qquad \widetilde{K}_{\text{m}} = \frac{K_{\text{m}}}{s_0} \\ &\lambda \equiv \frac{k_{\text{cat}}}{ks_0}, \qquad \epsilon = \frac{e_0}{s_0} \end{aligned} \qquad [22]$$

the corresponding chemical kinetic equations can be written as

$$\begin{aligned} \frac{d\tilde{s}}{d\tilde{t}} &= -\tilde{s} + \tilde{c}(\tilde{s} + \widetilde{K}_{\text{m}} - \lambda) \\ \epsilon\frac{\tilde{c}}{d\tilde{t}} &= g(\tilde{s},\tilde{c}) \equiv \tilde{s} - \tilde{c}(\tilde{s} + \widetilde{K}_{\text{m}}) \end{aligned} \qquad [23]$$

Noticing that $\epsilon \ll 1$ (the enzyme is present in infinitesimal quantities compared to the substrate), a quasistationary approximation applies for the variable $\tilde{c}$: it means that the intermediary species ES rapidly reaches a local equilibrium state $\tilde{c}=\tilde{c}^*(\tilde{s})$. This yields the substrate evolution

$$\frac{d\tilde{s}}{d\tilde{t}} = \frac{\lambda\tilde{s}}{\tilde{s} + \widetilde{K}_{\text{m}}} \qquad [24]$$

The initial condition is set only on the substrate: $s(0)=s_0$, that is, $\tilde{s}(0)=1$. It yields the well-known expression of the velocity $V\equiv (ds/dt)_{|t=0}$ as a function of the initial substrate concentration: $V(s_0)=e_0 k_{\text{cat}} s_0/(s_0+K_{\text{m}})$ (with a maximal value

$V_{\max} = e_0 k_{\text{cat}}$). The quasistationary value for the complex (dimensionless) concentration $\tilde{c}^*(\tilde{s}=1) = 1/(1+\tilde{K}_{\text{m}})$ at $t=0$ obviously differs from the actual initial condition $\tilde{c}(0)=0$: besides, it is quite foreseeable that the transients leading the complex *ES* to its stationary value cannot be described using a quasistationary approximation. At short times, the relevant time variable is the fast rescaled time $\theta = \tilde{t}/\epsilon$, leading to the equation describing the initial regime when supplemented with the actual initial condition $\tilde{c}(0)=0, \tilde{s}(0)=1$. The analysis is straightforwardly carried over, exactly as in the general abstract case, with a matching condition $\lim_{\theta\to\infty} \tilde{c}(\theta) = \tilde{c}(t=0) = 1/(1+\tilde{K}_{\text{m}})$.

Kinetic theory Time-matched expansions have been developed in kinetic theory, for instance, to describe the fate of a tagged particle within a gas. In a first, short stage (*kinetic stage*) following the injection of the particle in the thermally equilibrated gas, the velocity distribution of the particle rapidly evolves due to collisions with gas molecules and associated momentum transfer. This stage lasts a few mean-free-times and it ends when the tagged-particle distribution is almost Maxwellian. Then, in a second stage (*hydrodynamic stage*), the distribution slowly relaxes towards a spatially uniform distribution, ultimately equal to the equilibrium Maxwell–Boltzmann distribution; at each time, the velocity distribution is almost Maxwellian. The particle dynamics is described at the level of its distribution function by the Boltzmann equation, and the resolution (the so-called Chapman–Enskog method) is based on the above general principles.

The adiabatic-piston problem A matched two-timescale perturbation approach has been developed for the *adiabatic piston problem*: an isolated cylinder filled with an ideal gas (noninteracting light particles of mass m) is separated in two compartments by a moving piston, of mass M, adiabatic in the sense that it has no internal degrees of freedom and does not conduct heat when fixed. The small parameter is the mass ratio $\epsilon = 2m/(M+m)$. It quantifies the efficiency of energy transfer between the gas particles and the piston upon elastic collisions, and the strength of the indirect coupling of the two gas compartments through the collisions of their particles with one and the same piston. The matched perturbation approach gives access both to a fast deterministic relaxation towards mechanical equilibrium, at timescales $\mathcal{O}(1)$, with no heat transfer between the compartments, and a slow fluctuation-driven evolution towards thermal equilibrium, where the heat transfer is achieved by the collision-induced coupling between the gas and the piston fluctuating motion, thus occurring at timescales $\mathcal{O}(M/m)$ (*see* Adiabatic Piston).

Renormalization: An Iterated Multiscale Approach

It is not the place to expose or even summarize the implementation of renormalization techniques, for which we refer to the associated entries in this Encyclopedia. Here we will only stress the natural relations between renormalization group (RG) and multiscale approaches. The RG approach indeed shares many steps and guiding principles: joint rescalings, coarse-grainings and local averaging, effective parameters and effective terms, relevant and irrelevant contributions, with a focus on large-scale behavior. Moreover, far beyond the scope of the study of critical phenomena, RG has been extended into an *iterated multiscale approach* allowing to determine in a systematic and constructive way the effective equation describing the universal large-scale features and asymptotics of a multiscale system (see, e.g., Chen *et al.* (1996) and Mazzino *et al.* (2004).

It is first to be underlined that different meanings are associated with the term "renormalization," corresponding to very different statuses for the associated renormalization procedures.

A renormalized quantity can be plainly a *rescaled* quantity (normalized, dimensionless or put to the scale of the considered sample): here arises a first connection with multiscale approaches, both involving rescalings as an essential preliminary step.

A renormalized quantity can be an *effective quantity* accounting in an integrated way of complicated underlying mechanisms (e.g., the renormalized mass of a body moving in a fluid, accounting for hydrodynamic effects); here arises another central notion of multiscale approaches: effective parameters or effective equations (following, e.g., from averaging or homogenization).

Renormalization is also a mathematical technique developed first in celestial mechanics, and then mainly in quantum electrodynamics to *regularize* divergent expansions and perturbation series. It might proceed by means of *resummation*; the idea, implemented by Rayleigh in 1917, is to sum up correlations and interactions into a redefinition of the parameters. It might either rely on the introduction of a *cutoff* in the space, time, and energy scales, then accounting in an effective way of the host of contributions at smaller space and time scales $\Delta x \leq \Lambda$, $\Delta t \leq \theta$ (or, equivalently, larger momentum

and frequency scales: $k \geq 2\pi/\Lambda, \omega \geq 2\pi/\theta$) so as to take advantage of the physical cancellation of mathematical divergences. In any case, it turns the bare parameters of the original singular expansion into *renormalized parameters* and yields a renormalized regular expansion. Writing that the resulting large-scale behavior does not depend on the chosen cutoff (Λ, θ) yields *renormalization equations*, expressing quantitatively the very consistency of the procedure ("renormalizability" of the expansion). Renormalization provides alternative technical tools in instances treated above with the multiple-scale method. Its main advantage is its *recursive structure*: introducing a sequence $(\Lambda_n, \theta_n)_n$ of cutoffs (what is called momentum-shell RG), the whole procedure can be iterated to integrate recursively the influence of small-scale features on the asymptotic behavior, allowing as to handle situations exhibiting a hierarchy or even a continuum of scales.

Renormalization also refers to an *asymptotic analysis* allowing as to classify critical behaviors, to determine quantitatively the critical exponents and to handle the associated divergences. Indeed, the above-mentioned multiscale approaches fail near bifurcation points or critical points. In this case, scale separation is replaced by *scale invariance*. The key idea, underlying RG techniques is to shift the focus on the scaling procedure itself. The basic point is to construct a renormalization transformation, consisting in *joint coarse-grainings and rescalings*, thus relating the two models *describing the same phenomenon at different scales* (Lesne 1998); it puts forward their self-similar properties and associated scaling laws, while eliminating specific small-scale details having no consequences on the asymptotic, large-scale behavior. The set of renormalization transformations has a semigroup structure with respect to the rescaling factor (or plainly with respect to iteration) justifying to speak of RG. It generates a *flow in the space of models*, whose fixed points correspond either to trivial or to critical situations according to their stability. It can be shown that the linear analysis of the renormalization transformation around a critical fixed point gives access to the critical exponents. Moreover, this analysis allows us to split the space of models into *universality classes*, each associated to the basin of attraction of a critical fixed point. Let us emphasize that scale invariance leads to a deep change in the modeling and investigations, shifting from a "physics focusing on the prediction of amplitudes" to a "physics of the exponents," focusing on less specific, but more universal and above all, more intrinsic features.

Far more generally, RG is associated with a qualitative change in the questioning, since the study takes place in a space of models. Generalized renormalization transformation can be designed to extract not only self-similarity properties but any large-scale feature from a more microscopic model. In particular, RG can be specially designed to discriminate between essential and inessential terms in a model: the latter do not modify the asymptotics of the RG flow, meaning that they are of no consequence at large scales. In other words, generic properties of the renormalization flow in this space of models yield universal large-scale scaling properties. RG is thus essentially a multiscale approach, insofar as it only retains the relations between the different levels of descriptions, somehow ignoring the details at each given scale. *It is actually designed to capture universal features of the multiscale organization.*

Summary: The Exemplary Case of Diffusion

Bridging the Scales

Our aim in this section is to present the whole range of multiscale approaches in use, allowing both to bridge models devised at different scales and to predict the large-scale features of the phenomenon they account for. We choose the context of diffusion, Brownian motion, and transport phenomena, where such a bridge is essential and has been much investigated. Indeed, transport coefficients are defined through phenomenological equations; it is thus necessary to relate such macroscopic equations with smaller-scale theories, so as to get an expression of the coefficients in terms of the microscopic ingredients and to justify the validity of the phenomenological description.

The exposition in the various subsections below, following increasing scales, will mark out the pathway from reversible molecular dynamics to macroscopic diffusion equations. We shall thus come across the multiple-scale analysis of the Liouville equation describing at microscopic scales a Brownian grain suspended in a thermal bath of water molecules (see the next subsection) leading to the mesoscopic Kramers equation for the grain distribution function $P(r, v, t)$. Next, involving higher but still mesoscopic scales, we see that another multiple-scale analysis leads to the reduced Smoluchowski equation for its spatial distribution $P(r, t)$. Random walks offer alternative mesoscopic models, involving effective diffusion coefficients in order to take into account underlying features like persistence length or other short-range correlations. Scaling limits or more systematic renormalization methods in real space allow to bridge discrete random-walk models with continuous descriptions. Another RG, based on

a path-integral formulation in the framework of field theory, allows to handle the case of self-avoiding walks with infinite memory. Homogenization is illustrated on the case of diffusion in a regular porous medium, whereas diffusion processes in fractal substrates provide a counterexample, singular enough to exhibit anomalous scaling behavior. The issue of reducing the dynamics of the diffusion process to a simpler effective one is encountered in many other macroscopic instances, among which we shall mention diffusion in a periodic medium, lending to space averaging, and advection of a passive scalar field in a two-scale velocity field, where a multiple-scale analysis yields the effective diffusivity at large scale. We shall give further technical guidelines for constructing these steps climbing from molecular up to large macroscopic scales, thus providing additional illustrations of the multiscale approaches introduced in the previous sections on more general and abstract grounds.

Microscopic Theory of Brownian Motion

The first theoretical account of Brownian motion, namely the erratic movement of a micron-sized pollen grain suspended in a thermal bath, for example, water, dates back to 1905 and the famous paper by Einstein. It took almost 60 years before a *microscopic* theory was achieved; this theory has been further worked out using multiple-scale techniques (Cukier and Deutsch 1969). The challenge is to start from the complete deterministic reversible dynamics of the system, described within a probabilistic framework by the Liouville equation $\partial p/\partial t = Lp$ for the distribution of probability p in the whole phase space (position and velocities of the grain, of mass M, and all water molecules, of mass $m \ll M$). The small parameter is the mass ratio $\epsilon = \sqrt{m/M}$ measuring the efficiency of the energy transfer upon collisions between the grain and the bath particles, assuming a binary interaction potential $U = \sum_i u(|\boldsymbol{r}_i - \boldsymbol{r}|)$. The Liouville operator is decomposed into $L = L_0 + \epsilon L_1$, and one introduces rescaled time variables $\tau_n = \epsilon^n t$, where $\tau_0 = t$ is the timescale of the fluid particle dynamics. Multiple-scale method is carried out according to the general scheme, leading to the so-called Kramers equation,

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v}.\frac{\partial}{\partial \boldsymbol{r}}\right) P(\boldsymbol{r}, \boldsymbol{v}, t) = \zeta \frac{\partial}{\partial \boldsymbol{v}}\left[\boldsymbol{v} + \frac{kT}{M}\frac{\partial}{\partial \boldsymbol{v}}\right] P(\boldsymbol{r}, \boldsymbol{v}, t) \qquad [25]$$

where the friction coefficient is explicitly given as

$$\zeta = \frac{1}{3MkT}\int_0^\infty \langle \boldsymbol{F}_t.\boldsymbol{F}_0\rangle \, \mathrm{d}t \quad \text{where } \boldsymbol{F}_t = \mathrm{e}^{\mathrm{i}L_0 t}\boldsymbol{F}_0 \text{ and } \boldsymbol{F}_0 = -\nabla_{\boldsymbol{r}} U \qquad [26]$$

We refer to the original, although very pedagogical, paper by Cukier and Deutsch (1969) for a thorough exposition and discussion of this derivation.

Mesoscopic Theory of Brownian Motion

Multiple-scale method is also of relevance to determine the high-friction limit of the above Kramers equation. Standard perturbation technique with respect to the inverse of friction, $1/\zeta$, fails to describe the asymptotic regime: there is not enough freedom to fulfill all the solubility conditions required to avoid the appearance of secular divergences (Bocquet 1997). By contrast, multiple-scale technique yields a uniform expansion of the evolution equation still valid at long times, thus allowing to bridge two mesoscopic levels of description, namely the Kramers equation and the Smoluchowski equation for the spatial density $\rho(\boldsymbol{r}, t)$ of the Brownian particle:

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r}, t) = \frac{1}{M\zeta}\frac{\partial}{\partial \boldsymbol{r}}\left(kT\frac{\partial}{\partial \boldsymbol{r}}\right)\rho(\boldsymbol{r}, t) \qquad [27]$$

Introducing dimensionless variables $\tau = tv_{\mathrm{th}}/l, \boldsymbol{R} = \boldsymbol{r}/l, \boldsymbol{V} = \boldsymbol{v}/v_{\mathrm{th}}$, where l is the size and $v_{\mathrm{th}} = \sqrt{kT/M}$ the thermal velocity of the grain, the relevant small parameter appears to be the dimensionless inverse of the friction coefficient, $\epsilon = v_{\mathrm{th}}/l\zeta$; hence,

$$\epsilon\left(\frac{\partial}{\partial \tau} + \boldsymbol{V}.\frac{\partial}{\partial \boldsymbol{R}}\right) P(\boldsymbol{R}, \boldsymbol{V}, \tau) = \frac{\partial}{\partial \boldsymbol{V}}\left[\boldsymbol{V} + \frac{\partial}{\partial \boldsymbol{V}}\right] P(\boldsymbol{R}, \boldsymbol{V}, \tau) \qquad [28]$$

If the friction is high (i.e., $\epsilon \ll 1$), the velocity relaxes very rapidly towards the equilibrium Maxwell distribution, and it is then enough to describe the (slow) evolution of the spatial distribution $\rho(\boldsymbol{r}, t)$. Nevertheless, the relaxation stage is essential and accordingly the ϵ-dependence is singular, as a rule when the small perturbation parameter multiplies the time derivative.

According to the general procedure exposed in the section "Multiple-scale method: principles," we introduce rescaled variables $\tau_0 = \tau, \tau_1 = \epsilon\tau, \tau_2 = \epsilon^2\tau, \ldots$ considered as independent variables and look for a solution of the Kramers equation of the form $P = P^{(0)} + \epsilon P^{(1)} + \epsilon^2 P^{(2)} + \cdots$, where the arguments of all the components $P^{(i)}$ are $(\boldsymbol{R}, \boldsymbol{V}, \tau_0, \tau_1, \tau_2, \ldots)$. Identifying term-wise the successive powers of ϵ yields

a hierarchy of equations. At order 0, we obtain $P^{(0)} = \Phi(\boldsymbol{R}, \tau_0, \tau_1, \tau_2, \ldots)e^{-V^2/2}$. The following equations, for the $[P^{(i)}]_{i\geq 1}$, involve the linearized operator $\mathcal{L} = \partial_V(V + \partial_V)$. For each of them, there appears a solubility condition, requiring that none of the additive contributions in the equation is an eigenvector of $\mathcal{L}$; involving the components $P^{(j)}$ with $j < i$, it prevents the appearance of a secular divergence in $P^{(i)}$. At order[1], the solubility condition is $\partial\Phi/\partial\tau_0 = 0$, thus determining the (trivial) τ_0-dependence of $P^{(0)}$. In a similar way, the solubility condition at order 2 allows to determine the τ_1-dependence of $P^{(0)}$. This bridges the Kramers and Smoluchowski equations in the high-friction limit, when retaining only the first-order term in ϵ. We refer to Bocquet (1997) for a pedagogical account of the derivation and discussion of its relation with the time-derivative expansion involved in the so-called Chapman–Enskog solution of the Boltzmann equation.

Random-Walk Model and Weakly Correlated Diffusion

Random walks are discrete-time mesoscopic models, accounting for the diffusing motion of a particle through the statistical properties of its successive steps, when observed at a given timescale τ. The basic model (*ideal random walk*) assumes isotropic, independent and identically distributed steps of variance a^2. Central-limit theorem straightforwardly gives the time dependence of the mean-square displacement $R^2(t) \equiv \langle|\boldsymbol{r}(t) - \boldsymbol{r}(0)|^2\rangle = a^2t/\tau$, showing that the motion is a normal diffusion, with diffusion coefficient $D = a^2/2d\tau$ in dimension d. It is to note (see also the next subsection) that D depends τ and a, but in a *joint manner*. Actually, the diffusion coefficient associated with a diffusive motion observed at scale a and modeled by a random walk on a lattice of parameter a can be written as $D = \alpha a^2$, where the rate α depends on a (effective rate at spatial resolution a): this is a sort of renormalization that accounts for the rate $\alpha(a)$ of all microsteps backward and forward of length far smaller than a.

In case of short-range correlations between the successive steps (namely if $\sum_{-\infty}^{\infty}|C(t)| < \infty$, where $C(t)$ is the statistical correlation function between elementary steps separated by a time length t), direct computations support a time-average-like result: the asymptotic behavior is still described by a normal diffusion law $R^2(t) \sim 2dD_{\text{eff}}t$, with $D_{\text{eff}} = D\sum_{-\infty}^{\infty} C(t)$. When $C(t) = e^{-t/\tau}$

$$D_{\text{eff}} = \frac{D(1 + e^{-1/\tau})}{1 - e^{-1/\tau}}$$

hence $D_{\text{eff}} \approx 2\tau D$ if $\tau \ll 1$.

Renormalization Analysis in Case of Markovian Diffusion

Trying to bridge lattice random walks with a continuous description brings out the following difficulty: as the step size a goes to 0, one has to obviously decrease the duration τ accordingly, but by what amount is not so obvious, since the walker velocity is ill-defined (it depends on the observation scale). Determination of the proper joint rescaling can be guessed from the knowledge obtained by another mean about the system; rather, it can also be obtained in a systematic way, thanks to RG methods. Let us explain the basic principle.

Let us denote by $P_{a,\tau}(x, y, t)$ the transition probability governing the random walk, namely the density of probability to jump from x to y in time t, where x, y are restricted to the lattice $(a\mathbf{Z})^d$ and time to $\tau\mathbf{N}$. The renormalization transformation $\Phi_{k,\alpha}$ should express the consequence for $P_{a,\tau}$ of a joint rescaling of space (by a factor of k) and time (by a factor of k^α). Taking into account the Markov character of the walks, we are thus led to define

$$[\Phi_{k,\alpha}P_{a,\tau}](x, y, t) \equiv k^d P_{a,\tau}(kx, ky, k^\alpha t) \quad \text{in dimension } d \qquad [29]$$

The proper value of α is to be determined self-consistently in order that the limit $\lim_{k\to\infty} \Phi_{k,\alpha} P_{a,\tau}$ exists (it is then a continuous transition probability $P^*_\alpha(x, y, t)$ defined on $\mathbf{R}^d \times \mathbf{R}^d \times \mathbf{R}$). The root-mean-square displacement

$$R(P,\, t) \equiv \left[\sum_{x,y} |x - y|^2 P(x,\, y,\, t)\right]^{1/2}$$

is transformed according to

$$R(\Phi_{k,\alpha}P_{a,\tau}, t) = k^{-1}R(P_{a,\tau}, k^\alpha t) \qquad [30]$$

Accordingly, it yields the diffusion law associated with the fixed point P^*_α:

$$\text{for any } k,\ R(P^*_\alpha, t) = k^{-1}R(P^*_\alpha, k^\alpha t), \quad \text{hence } R(P^*_\alpha, t) \sim t^{1/\alpha} \qquad [31]$$

It is anomalous except if $\alpha = 2$. In the case of ideal random walks, the proper exponent leading to a nontrivial limit is $\alpha = 2$; this limit P^*_2 is the transition probability of a *Wiener process*:

$$W_D(x, y, t) = [4\pi dDt]^{-d/2} e^{-(x-y)^2/4dDt} \quad \text{with } D = a^2/2d\tau \qquad [32]$$

This shows that *all ideal lattice random walks belong to the same universality class*, that of the Wiener process. This approach has been fruitfully

applied to diffusion in disordered systems, the issue being to determine whether or not the disorder, accounted for as a noise term in the transition probabilities, modifies the normal diffusion law obtained in the unperturbed situation. Similar reasoning can also be implemented for self-similar anomalous diffusion processes, like *fractional Brownian motions* and *Levy flights* (Lesne 1998).

Renormalization Analysis for Self-Avoiding Walks

Let us only mention, for the sake of completeness, the renormalization techniques developed for determining the conformational statistics of linear polymer chains, whose three-dimensional shape can be represented as the trajectory of a self-avoiding random walk. These techniques belong to the RG corpus developed in statistical mechanics for critical phase transitions, within a field-theoretic framework. A formal but exact analogy can actually be worked out between self-avoiding walks and a spin lattice system with $n \to 0$, where n is the number of spin components.

The multiscale nature of the system is so marked here that it should rather be qualified as an *absence of characteristic scale*. In this respect, standard RG methods developed for critical phenomena lie at the very boundary of multiscale approaches. Scale decoupling is replaced by scale invariance, which is somehow the conjugate situation: homogeneity in real space is replaced by homogeneity in the conjugate space (space of characteristic scales). Scale invariance here reflects in the self-similar property, $R(N) \sim N^{\nu}$, relating the end-to-end distance R of the chain to the number N of elementary steps (the monomers), with an anomalous exponent ν (the Flory exponent $\nu \approx 3/5$ in dimension $d = 3$) originating from the infinite memory of the nonoverlapping chain. We refer to Lesne (1998) and references therein for a more detailed exposition of the concepts and techniques only alluded here.

Effective Diffusion in a Porous Medium (Homogenization)

Describing the diffusion in a porous medium appears as a formidable task at the pore level: it would require us to account for all the boundary conditions at the border of the hollow domain $\mathcal{V} \in \mathcal{V}_0$ actually accessible to diffusion. When the pores have a finite characteristic size a, a homogenization approach can be developed at scales far larger than a. It allows to account for the slowing down of the motion due to obstacles in an effective diffusion coefficient (in plain words, the black and white medium made of matter and holes of size a appears as a grey homogeneous medium at larger scales). More specifically, a diffusing tracer of random trajectory $r(t)$ experiences a varying coefficient $D[\boldsymbol{r}(t)]$ (it equals D inside the pores, whereas it vanishes in the nonaccessible region $\mathcal{V}_0 - \mathcal{V}$). The idea is to replace this fluctuating realization of the transport coefficient by its spatial average (independent of the trajectory), in what concerns macroscopic properties:

$$D_{\text{eff}} = \int_{\mathcal{V}_0} D\, n_0(\boldsymbol{r})\, \mathrm{d}^d\boldsymbol{r} = \int_{\mathcal{V}} D[\boldsymbol{r}]\, \mathrm{d}^d\boldsymbol{r}$$
$$(\text{where } n_0(\boldsymbol{r}) = 1 \text{ iff } \boldsymbol{r} \in \mathcal{V}) \qquad [33]$$

Rigorous mathematical theorems ensure that the large-scale motion can actually be described by a Fick law and associated plain diffusion equation (Bensoussan *et al.* 1978).

Anomalous Diffusion in a Fractal Medium

The above homogenization for diffusion in a porous medium works well only if the pores have a finite characteristic size; by contrast, diffusion in a fractal substrate (e.g., a porous medium with pores of all sizes) generically leads to anomalous diffusion, associated with a time dependence of the mean-square displacement $R^2(t) \sim t^{\gamma}$ with $\gamma < 1$. In a fractal substrate, the existence of obstacles and pores of all sizes introduces spatial fluctuations at all scales and long-range correlations in the spatial dependence of D. This case corresponds to a critical situation and homogenization fails to give a relevant description of the macroscopic behavior, in the same way as mean-field methods fail to account for critical phase transitions. It reflects in the anomalous exponent $\gamma < 1$ of the diffusion law, that can be related to the fractal characteristics of the substrate ($\gamma = d_s/d_f$, where d_s is the spectral dimension and d_f the fractal dimension).

Effective Diffusion in a Periodic Potential (Averaging Method)

In case of a periodic medium, where $D[\boldsymbol{r}(t)]$ oscillates with a small spatial period, an averaging procedure can be developed as in the subsection "Effective diffusion in a porous medium (homogenization)," to determine an effective diffusion equation accounting for the large-scale motion. Explicit computations within a multiple-scale approach yield

$$D_{\text{eff}} = \frac{1}{\langle D \rangle} \qquad [34]$$

where $\langle D \rangle$ denotes a space average over the elementary cell (Givon *et al.* 2004).

Let us rather detail the case of diffusion of a Brownian particle in a periodic potential U, with $U(x + L) = U(x)$ for any x (restricting to dimension 1 for simplicity), at equilibrium at temperature T. Let D be the coefficient of this particle in the

absence of the potential. At large scales $dx \gg L$, the substrate appears to be spatially uniform. The influence of the periodic bias exerted by the potential on the diffusive motion (superimposition of a modulated deterministic drift) can be described in an average way. The result is a normal diffusion with a reduced effective diffusion coefficient

$$D_{\text{eff}}(U) = D \inf_{f \in C^{\infty}(LS_1)} \int_0^L |1 - f'(x)|^2 \, dm_U(x)$$
$$\text{with } dm_U(x) = \frac{e^{-U(x)/kT} \, dx}{\int_0^L e^{-U(x')/kT} \, dx'} \qquad [35]$$

where the infimum is taken over the set of smooth periodic functions of period L and the average involves the equilibrium distribution m_U of the particle in the potential landscape $U(.)$. So doing, one sees in particular that no oriented motion can arise at equilibrium, even if U is asymmetric. The procedure extends to dimension d with only technical differences.

Effective Diffusivity for a Passively Advected Scalar

Still another fruitful implementation of multiple-scale method is encountered in the context of diffusion and transport phenomena, in the study of the advection by a given incompressible velocity field $\boldsymbol{v}(\boldsymbol{r}, t)$ of a passive scalar field $\theta(\boldsymbol{r}, t)$, for example, the density of small inert "tracer" particles advected by the fluid flow without modifying it back. We consider the case when the fluid motion can be decomposed into a large-scale, slowly varying component and a small-scale, rapidly varying fluctuation: $\boldsymbol{v}(\boldsymbol{r}, t) = \boldsymbol{U}(\boldsymbol{r}, t) + \lambda \boldsymbol{u}(\boldsymbol{r}, t)$. The parameter λ controls the relative strength of these components. Another small parameter λ is involved in this problem: the ratio $\epsilon = l/L \ll 1$ of the typical length scales L and l of $\boldsymbol{U}$ and $\boldsymbol{u}$, respectively. Here the issue is to bridge two macroscopic descriptions: the full hydrodynamic equation describing the evolution of the scalar field $\theta(\boldsymbol{r}, t)$

$$\frac{\partial}{\partial t}\theta(\boldsymbol{r}, t) + \boldsymbol{v}(\boldsymbol{r}, t).\nabla\theta(\boldsymbol{r}, t) = D\Delta\theta(\boldsymbol{r}, t) \qquad [36]$$

and a large-scale effective transport equation for an average scalar field $\theta_L(\boldsymbol{r}, t)$,

$$\frac{\partial}{\partial t}\theta_L(\boldsymbol{r}, t) + \boldsymbol{U}(\boldsymbol{r}, t).\nabla\theta_L(\boldsymbol{r}, t) = \frac{\partial}{\partial r_i}\left[D_{ij}^{\text{eff}} \frac{\partial}{\partial r_j}(\boldsymbol{r}, t)\theta_L(\boldsymbol{r}, t)\right] \qquad [37]$$

This procedure, amounting to account in an average way for the small-scale contributions to the complete hydrodynamic description, relies on a spatio-temporal generalization of the multiple-scale method: it involves rescaled space and time variables, $\boldsymbol{X} = \epsilon \boldsymbol{x}, \tau = \epsilon t, T = \epsilon^2 t$ The different characteristic scales of the velocity components are directly reflected in their arguments: $\boldsymbol{u}(\boldsymbol{x}, t)$ and $\boldsymbol{U}(\boldsymbol{X}, T)$. The passive scalar field now expresses $\theta(\boldsymbol{x}, t, \boldsymbol{X}, \tau, T)$ and it is expanded as $\theta = \theta^0 + \epsilon\theta^1 + \epsilon^2\theta^2$. The standard multiple-scale procedure leads to introduce an auxiliary field χ:

$$\partial_t\chi_j + [(\boldsymbol{u} + \lambda\boldsymbol{U}).\partial]\chi_j - D\,\partial^2\chi_j = -u_j \qquad [38]$$

yielding the effective diffusivity tensor (where $\langle\,\rangle$ is a space average)

$$D_{ij}^{\text{E}} \equiv \frac{D_{ij}^{\text{eff}} - D_{ji}^{\text{eff}}}{2} = D\sum_p \langle\partial_p\chi_i\partial_p\chi_j\rangle \qquad [39]$$

Advection enhances transport, and eddy diffusivity is larger than molecular diffusivity. In realistic cases, there is a continuum of scales $u = \sum_{n=0}^{N} u_n$, where u_n has a characteristic scale $l_n \sim 2^{-n} l_0$. Multiple-scale method is to be iterated into an RG analysis, achieving a recursive integration of the small and fast scales into D^{E} starting from the smallest and fastest ones.

Conclusions

Multiscale approaches allow to predict large-scale behavior generated by a given model; even more, they offer constructive tools to bridge models at different scales for the same phenomenon. They provide systematic and mathematically well-controlled tools to turn faithful but intractable models into effective reduced ones, thus lying at the core of statistical mechanics, many-body dynamical systems, and, more generally, at all issues of the still-in-progress complex systems science. Indeed, in a complex system (that might be their very definition), levels are so interrelated that it is essential to investigate jointly all the scales, from elementary units up to the whole system, and its emergent properties; neither theoretical nor numerical approaches can alone consider all the levels together, showing the relevance, if not the necessity, of multiscale approaches.

Basic preliminary issues are to determine the proper elementary level, the proper collective variables, and the relevant small parameters. Let us remark that the implementation of a multiscale technique rapidly faces the fundamental issue of defining a macroscopic variable; it offers some clues, indicating that a macroscopic variable might be a

phenomenological quantity observable at our scale, a slow mode, or collective variable.

Multiscale approaches take benefit of the separation of scales involved in the different mechanisms at work in the phenomenon under consideration. The basic idea, seen above at work in various instances and different ways, is to somehow decouple the different scales and to solve several simpler single-scale problems. Any multiscale implementation actually involves, at some stage and more or less explicitly, a limiting process in which the scale separation ratio $1/\epsilon$ tends to ∞: this limiting process has to be carefully controlled in order that the method can be applied to real situation. Finally, to be successful, multiscale approaches should achieve a trade-off between:

- *accuracy* (minimizing the loss of information involved in the reduction or projection technique),
- *efficiency and tractability* (this is, e.g., one of the major successes of hydrodynamics)
- *robustness* of the resulting reduced model (to be checked *a posteriori*),
- *flexibility* (extending to heterogeneous systems involving different components), and
- *scope* (bridging many different levels in order to capture the whole hierarchical structure).

Let us conclude by emphasizing a much fruitful benefit of multiscale approaches: they allow to investigate structural stability of a model, in particular to evidence relevant parameters and essential mechanisms controlling large-scale features. In this respect, they lead beyond the (necessarily restricted) scope of a specific model and give an explicit account of the observer biased view, related to its scale of observation. They hence contribute to capture a more complete and controlled understanding of the real physical systems.

Finally, a note on bibliographic guide to multiscale approaches may be useful. Technical details and several applications of multiscale perturbative expansions, in particular multiple-timescale method, with references to the original papers, can be found in Nayfeh (1973). Applications of multiple-scale method, fully worked out in a very pedagogical way, can be found in the work of Cukier and Deutsch (1969), Piasecki (1993), Bocquet (1997), and Mazzino *et al.* (2004). An acknowledged reference on homogenization techniques and multiscale analysis in periodic media is Bensoussan *et al.* (1978); see also the monographs by Lochak and Meunier (1988) and Berdichersky *et al.* (1999). Two recent review papers on multiscale approaches and reduction techniques are Givon *et al.* (2004) and Gorban *et al.* (2004). Basic principles and technical aspects of scaling theories and RG approaches from a multiscale viewpoint can be found in Lesne (1998).

See also: Adiabatic Piston; Averaging Methods; Bifurcations in Fluid Dynamics; Boltzmann Equation (Classical and Quantum); Central Manifolds, Normal Forms; Interacting Particle Systems and Hydrodynamic Equations; Korteweg–de Vries Equation and Other Modulation Equations; Localization for Quasiperiodic Potentials; Singularity and Bifurcation Theory; Stability Problems in Celestial Mechanics; Stationary Phase Approximation; Universality and Renormalization.

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Negative Refraction and Subdiffraction Imaging

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Introduction

The concept of negative refraction has caused a revolution in classical optics and electromagnetic theory in the past few years (Pendry 2004, Ramakrishna 2005). If a material has negative dielectric permittivity (ε) and negative magnetic permeability (μ) simultaneously at a given frequency ω, then it can be said to have a negative refractive index defined as

$$n = -\sqrt{\varepsilon\mu} \qquad [1]$$

Several peculiar consequences of Maxwell's equations for the propagation of radiation in such a material were originally pointed out by Veselago (1968). But the lack of such natural materials failed to create much enthusiasm until recently when composite structured photonic materials have been shown to have negative refractive index (Smith *et al.* 2000, Shelby *et al.* 2001).

The question then boils down to what constitutes materials with negative ε and μ? Where the structure varies spatially on a scale much less than the wavelength of the incident radiation, composite electromagnetic materials can be regarded effectively as homogeneous media. A set of effective response functions: the effective permittivity, ε_{eff}, and the effective permeability, μ_{eff}, can then be ascribed to these materials. To develop a homogeneous view of the electromagnetic properties of a medium composed of discrete atoms and molecules was the motivation for defining a permittivity ε and permeability μ. The simplicity provided by such a description cannot be understated. Provided the radiation cannot resolve the underlying structure, replicating the atoms of a material with structure on a larger scale therefore represents a straightforward extension of the original concept.

If we consider arrays of structures defined by a unit cell of dimensions, d, then our effective description of the response of the medium to electromagnetic radiation of angular frequency ω will be valid provided that

$$d \ll \lambda = 2\pi c/\omega \qquad [2]$$

This restriction ensures that the underlying structure of the medium will merely refract and not scatter the incident radiation, in which case an effective permittivity and permeability for the medium become valid. The above inequality defines the long wavelength or effective medium limit (Garland and Tanner 1978). Maxwell's equations, written in the absence of free charges and external currents,

$$\nabla \cdot \boldsymbol{D} = 0, \qquad \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \qquad [3]$$

$$\nabla \cdot \boldsymbol{B} = 0, \qquad \nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} \qquad [4]$$

together with the constitutive relations:

$$\boldsymbol{B}(\omega) = \mu_0\mu_{\text{eff}}(\omega)\boldsymbol{H}(\omega) \qquad [5]$$

$$\boldsymbol{D}(\omega) = \varepsilon_0\varepsilon_{\text{eff}}(\omega)\boldsymbol{E}(\omega) \qquad [6]$$

then provide us with a complete description of the electromagnetic properties of the material over the frequency range of interest. Note that the effective-medium parameters are a function of the frequency as the material polarization response depends on the time history of the applied fields (Landau *et al.* 1984). These effective parameters were then generalized to analytic complex functions to account for absorption, and to second-ranked tensors to describe anisotropic responses.

The real parts of these effective material parameters can always be negative; there is nothing fundamentally wrong about that. Provided that they are dispersive, that is, they vary as a function of frequency, and dissipative as a consequence of the famous Kramers–Kronig relations (Landau *et al.* 1984), such materials are causally possible. Simultaneously negative values of ε_{eff} and μ_{eff} change the nature of electromagnetic radiation in these media.

For example, the wave vector in such isotropic media points opposite to the Poynting vector and gives rise to many new interesting effects such as modified refraction, negative Doppler shifts, etc. Such materials can support a variety of surface electromagnetic modes, which can have dramatic effects such as the possibility of a perfect lens which has unlimited image resolution (Pendry 2000) and is not subject to the traditional diffraction limit.

New artificial electromagnetic composite structures, often referred to as "meta-materials," allow us to access values of these material parameters which are not found in naturally occurring materials. We will show here how to obtain negative values of ε_{eff} and μ_{eff} in meta-materials using a variety of resonance phenomena. Then we will look at the problem of imaging with subdiffraction resolution using negative refractive index materials.

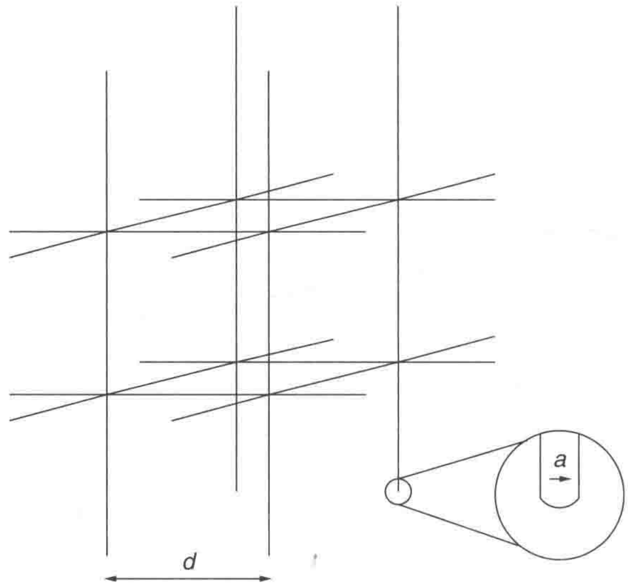


Figure 1 A periodic structure composed of infinite conducting wires arranged in a simple cubic lattice. Provided the factor a/d is small enough, the structure responds to incident electromagnetic waves as a plasma of very heavy charged particles.

Artificial Plasmas

From the electromagnetic viewpoint, a plasma can be represented as a medium with dielectric permittivity whose real part is negative. The Coulomb force and the finite mass of the electrons combine to give an ideal plasma a dispersion in the relative permittivity, $\tilde{\varepsilon}(\omega)$, given by

$$\tilde{\varepsilon}(\omega) = 1 - \frac{\omega_{\text{p}}^2}{\omega^2} \qquad [7]$$

where the plasma frequency is defined by $\omega_{\text{p}}^2 = (\rho e^2)/(\varepsilon_0 m_{\text{e}})$, ρ is the number density of electrons, e is the electronic charge, and m_{e} is the electron mass. The permittivity of the plasma is negative at frequencies below the plasma frequency.

A plasma-like behavior characterizes the electron gas in the noble and alkali metals, with a plasma frequency typically at ultraviolet frequencies. Because of the presence of dissipation, at lower frequencies resistive effects dominate and the plasmons cannot be excited. To obtain materials with negative dielectric permittivity at low frequencies, a lower plasma frequency is required corresponding to more massive particles and a lower particle density ρ. A structure consisting of a three-dimensional lattice of very thin wires simulates a low-density plasma of very heavy charged particles and is shown in **Figure 1** (Pendry *et al.* 1998). A simple model allows us to describe the desired reduction in ω_{p} in such a structure.

First consider a displacement of the electrons in the wires along one of the cubic axes. Only the wires directed along that axis are active and thus provide a lowered effective density of electrons, ρ_{eff}, given by the area occupied by the active wires. Thus,

$$\rho_{\text{eff}} = \rho \frac{\pi a^2}{d^2} \qquad [8]$$

An even more profound effect of constraining the electrons to run along thin wires is a result of the induced magnetic field which wraps the wires as the electrons are in motion. Suppose a current I flows in the wires. The magnetic field is

$$H(r) = \frac{I}{2\pi R} = \frac{\rho a^2 v e}{2R} \qquad [9]$$

where R is the distance from the wire center, v is the electron drift velocity, and ρe is the charge density in the wire. In terms of the magnetic vector potential, the magnetic field is

$$\boldsymbol{H}(R) = \mu_0^{-1} \boldsymbol{\nabla} \times \boldsymbol{A}(R) \qquad [10]$$

where

$$A(R) = \frac{\mu_0 a^2 \rho v e}{2} \ln(d/a) \qquad [11]$$

and d is the lattice spacing. The importance of the divergence of the magnetic field with the wire radius as seen in eqn [9] is the contribution to the canonical electronic momentum given by $e\boldsymbol{A}$. If we neglect the variation of the fields with distance from the wire center, we can view this contribution as defining a new effective mass for the electrons given by

$$m_{\text{eff}} = \frac{\mu_0 e^2 \rho}{2\pi} \ln(d/a) \qquad [12]$$

Now the effective plasma frequency for the system

$$\omega_{\mathrm{p}}^2 = \frac{\rho_{\mathrm{eff}} e^2}{\varepsilon_0 m_{\mathrm{eff}}} = \frac{2\pi c_0^2}{d^2 \ln(d/a)} \quad [13]$$

is seen to be much reduced. As an example, the plasma frequency of 1 μm aluminum wires paced by 10 mm is about 2 GHz, and the corresponding electronic effective mass is almost 15 times that of a proton! The factors of effective mass and charge density cancel leaving an expression comprising only the macroscopic system parameters. This is to be expected as a circuit analysis in terms of a capacitance and inductance can also be used to formulate the problem. However, such an approach can obscure the true nature of the problem which is encapsulated as a low-frequency plasma oscillation. Inclusion of the finite resistivity of the metal yields a finite lifetime for the plasmon excitation. Experiments have shown that a reduction in the plasma frequency of six orders of magnitude from the ultraviolet to the microwave region can be achieved in these thin-wire composites (Pendry *et al.* 1998).

Artificial Magnetism

Although the Maxwell equations [2]–[4] are symmetric in the electric and magnetic fields, we are yet to discover a free magnetic pole. The magnetism we find in natural materials is limited to spin systems and restricts the values of μ_{eff}. Up to microwave frequencies, magnetic activity is common and certain insulating ferromagnets and antiferromagnetic compounds such as MgF_2 and FeF_2 can even exhibit a negative permeability at some frequencies. However, large losses can accompany the magnetic activity in these materials.

Recently, it has become clear that a wide variety of composite structures comprising resonant inclusions can display magnetic activity in the effective medium limit (Pendry *et al.* 1999). Efficient screening of AC magnetic fields can be achieved using a thin cylindrical shell of metal or superconductor. In order to obtain a large magnetic response such that the modulus of the magnetic susceptibility, $|\chi_{\mathrm{m}}| > 1$, what we require is a resonant over-screening material response. A collection of subwavelength-sized structures that exhibits such an over-screening response can constitute a negative μ_{eff} material. One such resonant subwavelength structure is the so-called split-ring resonator (SRR), which can be scaled to form magnetic meta-materials from microwave to optical frequencies (Pendry *et al.* 1999, O'Brien and Pendry 2002b). An SRR structure which has been demonstrated experimentally to have a resonant magnetic response at microwave and THz frequencies is depicted in **Figure 2a** (Smith *et al.*). It comprises of two planar rings of metal on an insulating backing. The rings couple inductively to the magnetic field normal to the plane of the rings. Because of the large capacitance between the rings, the structure resonates at some frequency. Driven by the back electromotive force (emf), a large response is expected in the vicinity of the resonance frequency which is also antiphased in a small frequency range above the resonant frequency. If the SRRs are much smaller than the free-space wavelength, a collection of such SRRs would behave as a negative μ_{eff} material at these frequencies.

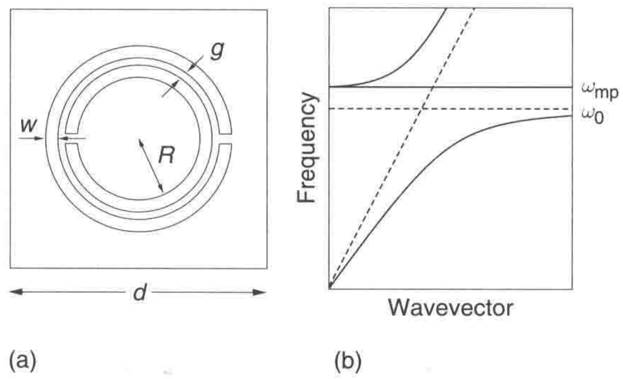


Figure 2 (a) The split-ring resonator structure. The structure is planar with an internal radius *R*. The metal rings are of width *w* and are separated by a spacing *g*. (b) Generic dispersion relationship, ω vs. *k*, for a resonant structure with an isotropic effective permeability as in eqn [15].

Theoretical calculations (Pendry *et al.* 1999) assuming a nondispersive metal show that a periodic lattice of such structures is characterized by a magnetic permeability given by

$$\tilde{\mu}_{\mathrm{eff}} = 1 - \frac{f\omega^2}{\omega^2 - \omega_0^2 + \mathrm{i}\Gamma\omega} \quad [14]$$

where $f = \pi R^2/d^2$ is the filling factor,

$$\omega_0 = \sqrt{\frac{3lc^2}{\pi R^3 \ln 2w/g}} \quad [15]$$

is the resonant frequency, and the damping of the resonance is determined by the factor

$$\Gamma = \frac{2l}{\mu_0 \sigma R} \quad [16]$$

Here *d* is the lattice spacing, *R* is the inner radius of the ring, *w* is the width of the rings, *l* is the distance between adjacent planes of SRRs, and σ is the conductance per unit length of the rings measured along the circumference. Orientation of planar SRRs

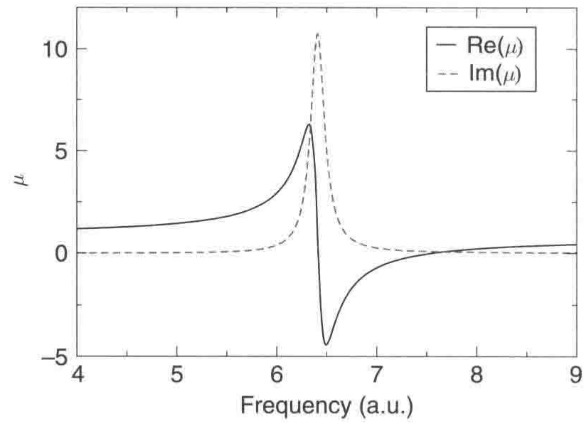


Figure 3 (a) The generic magnetic response of the SRR structure. Re(μ) < 0 in a frequency band above the resonance frequency.

along all three Cartesian axes allows for the creation of an isotropic material. **Figure 3** shows the generic dispersion of the $\mu(\omega)$ given by eqn [14]. A higher resistivity for the material of the SRR would broaden the resonance and the frequency region with Re(μ) < 0 might vanish altogether for large resistivity.

For isotropic homogeneous materials with a resonant effective permeability as in eqn [14] we can illustrate a generic dispersion relationship, ω vs. k, shown in **Figure 2b**. The solid lines represent twofold degenerate transverse modes and the dispersionless longitudinal magnetic plasmon mode at the magnetic plasmon frequency (ω_{mp}). The dashed lines are a band of propagating states with a linear dispersion determined by the polarizability of the SRRs and a flat band of resonant states at the magnetic resonance frequency ω_0. The gap in the dispersion can be regarded as arising from the hybridization and avoided crossing of these bands. The important points to note are:

1. Wherever μ_{eff} is negative there is a gap in the dispersion relationship. This is the case for $\omega_0 < \omega < \omega_{mp}$, the frequency where $\mu_{eff} = 0$. Only evanescent modes with imaginary wave vector exist in this region.
2. A longitudinal magnetic plasma mode, which shows no dispersion, appears at $\omega = \omega_{mp}$.

An alternative approach to obtaining a nonzero magnetic susceptibility in composite media is provided by the zeroth-order transverse electric (TE) Mie resonance in dielectric particles. Ferroelectric and phonon polaritonic materials are promising candidates for providing the necessary large dielectric constants up to infrared frequencies (O'Brien and Pendry 2002a).

The high-frequency scaling properties of the SRR offer an interesting insight. The plasma-like dielectric permittivity of noble metals

$$\tilde{\varepsilon}(\omega) = (\varepsilon_1, \varepsilon_2) = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \qquad [17]$$

is essentially a large negative real number for $\omega_p \gg \omega \gg \gamma$. For a 2D array of simplified SRRs consisting of a single conducting ring with symmetrically placed small capacitive gaps, the quasistatic effective magnetic permeability for a magnetic field applied normal to the plane of the SRR is (O'Brien and Pendry 2002b)

$$\tilde{\mu}_{eff} = 1 - \frac{f'\omega^2}{\omega^2 - {\omega_0}^2 + i\Gamma\omega} \qquad [18]$$

where $f' = L_g f \cdot (L_g + L_i)^{-1}, \Gamma = L_i\gamma \cdot (L_g + L_i)^{-1}$, and ${\omega_0}^2 = (L_g + L_i)^{-1}C^{-1}$. In the above expressions, $L_g = \mu_0 \pi R^2$ is the geometrical inductance per unit length of the structure and $C = \varepsilon_0 \tilde{\varepsilon}_s \tau / n_c d_c$ is the capacitance per unit length of the structure for series connection. Here it has been assumed that the thickness of the SRR (τ) is small compared to the skin depth $\delta \simeq c_0/\omega_p$.

An additional inductive impedance in the structure, the kinetic or inertial inductance, $L_i = 2\pi R/\varepsilon_0 \omega_p^2 \tau = 2\mu_0 \pi R \delta^2/\tau$, determines the effective filling fraction and damping of the resonance through the ratio of the two contributions to the total inductance. This contribution to the inductance arises from the finite electron mass and implies that simply decreasing the size of the resonators indefinitely will not result in our being able to realize a strong magnetic response at near-infrared or optical frequencies. As the dimensions of the structure are reduced that fraction of the energy of the displacement current associated with the inertial mass of the electrons increases. A finite γ then means that dissipative losses increase. Thus, strong damping of the resonance will be avoided if the quantity $R\tau/2\delta^2$ is large. We note here that with δ equal to the London penetration depth, this ratio also determines the screening efficiency of low-frequency magnetic fields by a thin layer of superconductor. This result points to a broader similarity between the low-frequency electromagnetic properties of the superconducting condensate and those of a perfect plasma.

Other nanocomposites in addition to the SRR have been proposed which may lead to a magnetic response at optical frequencies. These include pairs of nanometer-sized metallic sticks where simultaneous electric and magnetic dipole resonances lead to a strongly dispersive effective permittivity and permeability.

Negative Refractive Index Media

Interleaving the structures for a negative $\varepsilon_{\mathrm{eff}}$ and μ_{eff} can create a composite with $\varepsilon_{\mathrm{eff}} < 0$ and $\mu_{\mathrm{eff}} < 0$ at a common frequency (ω) (Smith *et al.*, Shelby *et al.* 2001), which as predicted by Veselago (1968) should give rise to a material with negative refractive index. Although this appears intuitively correct, it is actually nontrivial that the electromagnetic fields of the two composites do not interfere with each other's function (Pokrovsky and Efros 2002) and this could depend crucially on the relative placement of the two structures (Marques and Smith 2004). However, there is now overwhelming experimental and numerical evidence that such composite structures possess negative refractive index (see Ramakrishna (2005, section 6)). Now consider a medium with predominantly real ε and μ. For $\varepsilon > 0$ and $\mu > 0$, we have our usual optical materials. Only one of ε or μ lesser than zero with the other positive would imply a medium which cannot support any propagating modes. This is a consequence of Maxwell's equations:

$$\boldsymbol{k} \cdot \boldsymbol{k} = \varepsilon(\omega)\mu(\omega)\frac{\omega^2}{c_0^2} \qquad [19]$$

which implies that only evanescently decaying waves with an imaginary component of $\boldsymbol{k}$ are possible. Common examples are ordinary metals with $\varepsilon < 0$ and $\mu > 0$. Now consider a medium with both $\varepsilon < 0$ and $\mu < 0$, or a negative refractive index medium. The Maxwell's equations for a plane time-harmonic wave $\exp[\mathrm{i}(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)]$ are:

$$\boldsymbol{k} \times \boldsymbol{E} = \frac{\omega}{c}\mu(\omega)\boldsymbol{H} \qquad [20]$$

$$\boldsymbol{k} \times \boldsymbol{H} = -\frac{\omega}{c}\varepsilon(\omega)\boldsymbol{E} \qquad [21]$$

The "left-handedness" of the triad $(\boldsymbol{E}, \boldsymbol{H}, \boldsymbol{k})$ is clear from these equations for $\varepsilon(\omega)$, $\mu(\omega) < 0$. A real refractive index means that waves propagate with the direction of energy flow given by the Poynting vector,

$$\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H} \qquad [22]$$

opposite to the direction of the wave vector. Since the group velocity is in the direction of the energy flow, we conclude that in these left-handed materials (LHMs) the group velocity and the phase velocity are oppositely directed. The phase accumulated in propagating a distance x is $\Delta\phi = -\sqrt{\varepsilon\mu}\omega/c_0 x$. Thus, the refractive index can be taken to be $n = -\sqrt{\varepsilon\mu}$, that is, a negative quantity. Mathematically, it is more reasonable to ask for the sign of the square-root to determine the wave vector given by eqn [19]. It can be shown by arguments of analytic continuity in the complex plane that the negative sign has to be chosen for propagating waves when $\mathrm{Re}(\varepsilon) < 0$ and $\mathrm{Re}(\mu) < 0$ (Ramakrishna 2005).

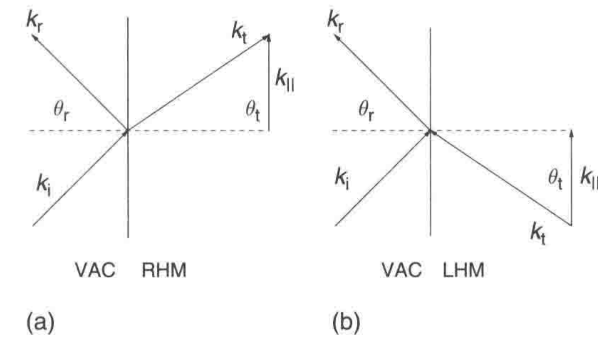


Figure 4 Illustration of Snell's law at an interface between two media with (a) positive refractive index (VAC/RHM) and (b) negative refractive index (VAC/LHM). The arrows indicate the wave vectors and the energy flow is opposite to the wave vector in the negative index medium.

The negative refractive index has real effects on the behavior of radiation even in basic processes such as refraction. Consider an interface between vacuum and a negative refractive index medium with $n < 0$ shown in **Figure 4**. Continuity conditions on the electromagnetic fields at the interface require for a plane wave incident from the vacuum side at an oblique angle that the parallel wave vector $k_{\|}$ is conserved for the transmitted and reflected wave. This is the origin of Snell's law:

$$\sin(\theta_\mathrm{i}) = \sin(\theta_\mathrm{r}) = n_- \sin(\theta_\mathrm{t}) \qquad [23]$$

where θ_i, θ_r and θ_t are the angles of incidence, reflection, and transmission, respectively. The flow of energy across the interface determines the direction of the group velocity in the material medium as being away from the interface. Therefore, the component of the phase velocity vector normal to the interface must change sign as we pass from vacuum into the material medium. We are then forced to conclude that the ray is bent toward the same side of the surface normal as the incident wave. This picture is consistent with Snell's law with the interpretation that $n < 0 \Rightarrow \theta_\mathrm{t} < 0$. **Figure 4** illustrates this point which has been experimentally verified by several groups (Shelby *et al.* 2001, Parazzoli *et al.* 2003, Eleftheriades *et al.* 2002).

As a direct consequence of this, it is seen that a flat slab of negative refractive medium can act as a lens as shown in **Figure 5**. Provided that the slab is of sufficient thickness, the refracted rays from a point source come to a focus inside the slab and upon exiting the slab the rays are redirected again such that they come to a focus on the opposite side of the slab (Veselago 1968). Veselago also predicted a negative Doppler shift in such media and an obtuse angle cone for Cerenkov radiation.

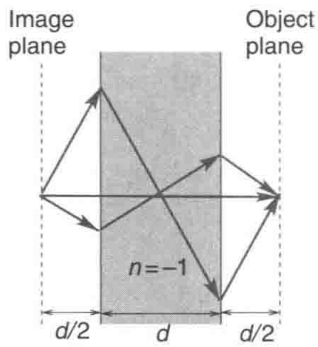


Figure 5 Steady-state passage of rays (representing the energy flow) of light from vacuum through a slab made of a LHM with $n=-1$. The slab acts as a lens mapping a point on the image plane to a point on the object plane.

Perfect Lens: Subwavelength Imaging

A wave analysis of the Veselago lens revealed an extremely novel aspect: it did not suffer from the diffraction limit and the image resolution could be infinite (Pendry 2000), if the negative index material were perfectly nondispersive and nonabsorbing. Before we analyze this, let us first briefly review the problem of imaging and the diffraction limit.

Any object is visible because it emits or scatters light. The problem of imaging is then concerned with reproducing the electromagnetic field distribution on a 2D object plane in the 2D image plane. If $E(x,y,0)$ be the electric field on the object ($z=0$) plane, the fields in free space can be decomposed into the Fourier components k_x and k_y, and polarization defined by σ:

$$E(x,y,z;t)=\sum_{\sigma,k_x,k_y} E_\sigma(k_x,k_y) \times \exp[\mathrm{i}(k_x x+k_y y+k_z z-\omega t)] \qquad [24]$$

where

$$E_\sigma(k_x,k_y)=\int_{x,y} E_\sigma(x,y,0)\,\mathrm{e}^{-\mathrm{i}(k_x x+k_y y)}\,\mathrm{d}x\,\mathrm{d}y \qquad [25]$$

In the above expression, the source is assumed to be monochromatic of frequency ω, $k_x^2+k_y^2+k_z^2=\omega^2/c_0^2$, c_0 is the speed of light in free space, and z is the optical axis. A conventional lens acts by applying a phase correction to each of the propagating components so that they reassemble to a focus at a point beyond the lens. For these components k_z is real, thus a phase change is all that is required to form an image containing these components. The higher spatial details in an object, however, are described by the nonpropagating near-field components with an imaginary k_z where $k_x^2+k_y^2>\omega^2/c^2$. A conventional lens cannot restore these components in the image plane as they decay exponentially in amplitude as one moves away from the source. Hence the resolution, Δ, provided by a conventional lens is limited to those components with

$$k_x^2+k_y^2<\omega^2/c^2 \Rightarrow \Delta \sim \frac{2\pi c}{\omega}=\lambda \qquad [26]$$

Now consider the slab of medium with $\varepsilon=-1$ and $\mu=-1$ and of thickness d_s. It can be shown (Pendry 2000) that the transmission and reflection coefficients are

$$\lim_{\substack{\varepsilon\to-1\\ \mu\to-1}} \tilde{t}=\exp[-\mathrm{i}k_z d_s] \qquad [27]$$

$$\lim_{\substack{\varepsilon\to-1\\ \mu\to-1}} \tilde{r}=0 \qquad [28]$$

respectively, where k_z is the component of the wave vector normal to the interface. Thus, the slab reverses the phase advance for the propagating waves as revealed by the ray picture. Analytic continuation to imaginary wave vectors $k_z=\mathrm{i}\kappa_z$ implies that the transmittance $\tilde{t}\to\exp(+\kappa_z d)$, that is, the slab also increases the amplitude of the evanescent waves in transmission at exactly the same rate as the rate of the decay in free space outside. Thus, each wave, propagating or evanescent, arrives at the image plane with its phase or amplitude restored exactly to the values at the object plane so as to perfectly reconstruct the image. The lens is also perfectly impedance matched and has zero reflection. These incredible properties have led the phenomenon to be called "perfect lensing."

Note that there is no energy flux associated with purely evanescent waves, and hence the amplification obtained in the steady state corresponds to local field enhancements which would imply the presence of localized resonances. In fact, the entire mechanism of the focusing of the near-field components is due to surface modes that reside on the surfaces of these negative index materials (Ramakrishna 2005). $\varepsilon=-1$ and $\mu=-1$ are precisely the conditions for these surface modes of electric and magnetic nature, respectively. These surface plasmon resonances which are excited resonantly by the evanescent modes and the secret to the perfect lens is that all the surface modes are completely degenerate.

Although the conditions for realizing a perfect lens are easy to specify, in practice these are very difficult to meet. The requirement of negative values for ε and μ implies that these quantities must disperse necessarily with frequency and be dissipative. Thus, the perfect-lens condition can only be met approximately at a single frequency. Any deviation from the ideal

conditions can then result in the excitation of slab polariton resonances which can swamp the image. The effects of absorption, which are always present, can also seriously degrade the lens performance by damping out the surface plasmon resonances (Ramakrishna 2005). Consider the transmission for the P-polarized radiation through a negative index slab:

$$\tilde{t}(k_x) = \frac{4(k_{z1}/\varepsilon_+)(k_{z2}/\varepsilon_-)\,e^{ik_{z2}d_s}}{\mathcal{D}} \qquad [29]$$

where

$$\mathcal{D} = (k_{z1}/\varepsilon_+ + k_{z2}/\varepsilon_-)^2 - (k_{z1}/\varepsilon_+ - k_{z2}/\varepsilon_-)^2 e^{2ik_{z2}d_s}$$

Under the perfect-lens conditions, the first term in the denominator goes to zero for evanescent waves and the exponential in the second term decays faster than the exponential in the numerator. However, if there was a mismatch in the conditions, ($\varepsilon_+ = 1$ and $\varepsilon_- = -1 + \delta$, say) then the first term in the denominator no longer vanishes. In the large wave vector limit ($k_x \gg \omega/c_0$), the two terms in the denominator become approximately equal when

$$k_x = -\frac{1}{d_s}\ln\left|\frac{\delta}{2}\right| \qquad [30]$$

thus yielding a criterion for the largest wave vector for which there is effective amplification. The dependence through the logarithm on the deviations (whether real or imaginary) from the resonant conditions underlines the fact that the perfect lens effect is indeed very sensitive. In practice, the periodicity, d, of the strucuture of the metamaterials comprising the negative index slab itself imposes an upper wave vector cutoff $k_c = 2\pi/d$. The material will become spatially dispersive for wave vectors $k \to k_c$, and for $k > k_c$ the very description as a homogeneous material will break down.

An important simplification of the perfect-lens conditions results when we consider a situation in which all length scales in the problem are much less than the wavelength of the light (the quasistatic approximation). Under these conditions, the electric and magnetic fields effectively decouple. If we consider the case of P-polarized fields, it can be shown (Pendry 2000) that in the quasistatic limit only the value of the permittivity is important, and there are essentially no conditions on the value of the permeability. This brings metals such as silver into the picture as the permittivity of silver becomes equal to –1 in the optical region of the spectrum and with relatively small losses (Pendry 2000). To overcome the losses, a series of refinements of the simple thin-slab picture have been proposed including dividing the lens into a series of layers and using optical amplification to act against the deleterious effects of absorption (Ramakrishna 2005).

The Generalized Perfect-Lens Theorem

The negative refractive slab can be considered as "optical antimatter" in the sense that it cancels out the effects on radiation of the traversal through an equal amount of positive refractive index medium. This cancelation is applicable to the phase changes for the propagating modes and the amplitude changes to the evanescent modes. In fact, the focussing action can happen for more general situations where the requirement of homogeneity of the slab material can be relaxed. Now consider the more general situation where the dielectric permittivity and the magnetic permeability are arbitrary functions of the spatial coordinates:

$$\varepsilon_+ = \varepsilon(x,y), \qquad \mu_+ = \mu(x,y) \qquad [31]$$

$$\varepsilon_- = -\varepsilon(x,y), \qquad \mu_- = -\mu(x,y) \qquad [32]$$

corresponding to the **Figure 6**. We will consider the imaging axis to be the z-axis. Thus, we see that the system is antisymmetric with respect to the $z = d$ plane. It turns out (Pendry and Ramakrishna 2003) that such a system also transfers the image of a source placed at the $z = 0$ to the $z = 2d$ plane in the same exact sense that it includes both the propagating and evanescent components. In general, the rays in spatially varying media will not be straight lines as shown in **Figure 6**, but the effect of propagating through the positive medium is nullified by the negative medium. Thus, to an observer on the right-hand side, it would appear as if the region between $z = 0$ and $z = 2d$ did not exist. We will call such media with the same sense of transverse spatial variation but with opposite signs as optical complementary media, and the effect of any such pairs of complementary media on radiation is null.

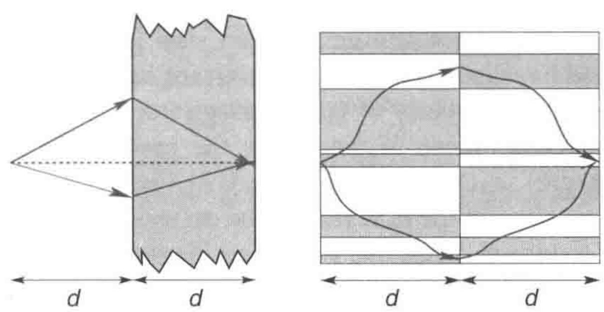


Figure 6 A pair of complementary optical media nullify the effect of each other for the passage of light. Spatially varying positive and negative refractive indices are schematically depicted by the white or shaded regions.

The most general conditions on the permittivity and permeability tensors for such complementary behavior are:

$$\tilde{\varepsilon}_+ = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$
$$\tilde{\mu}_+ = \begin{pmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{pmatrix} \quad [33]$$

and

$$\tilde{\varepsilon}_- = \begin{pmatrix} -\varepsilon_{xx} & -\varepsilon_{xy} & +\varepsilon_{xz} \\ -\varepsilon_{yx} & -\varepsilon_{yy} & +\varepsilon_{yz} \\ +\varepsilon_{zx} & +\varepsilon_{zy} & -\varepsilon_{zz} \end{pmatrix}$$
$$\tilde{\mu}_- = \begin{pmatrix} -\mu_{xx} & -\mu_{xy} & +\mu_{xz} \\ -\mu_{yx} & -\mu_{yy} & +\mu_{yz} \\ +\mu_{zx} & +\mu_{zy} & -\mu_{zz} \end{pmatrix} \quad [34]$$

and a perfect focus results whenever the two slabs of positive and negative media have such a behavior (see Pendry and Ramakrishna (2003) and Ramakrishna (2005) for the proof). This theorem clearly shows that the dependence along the x- and y-directions transverse to the imaging axis z is completely irrelevant as long as the two slabs are optically complementary. As an extension, it can be shown that any system of optically complementary media will also have a perfect focus as long as the system has a plane of antisymmetry normal to the optical axis. The above effects have also been numerically verified for several such spatially varying complementary media (Pendry and Ramakrishna 2003).

Perfect Lens in Other Geometries

The above generalized perfect-lens theorem along with a method of coordinate transformations can enable us to now generate a variety of superlenses in different geometries. In general, if we can find a geometric transformation that maps a given configuration into the geometry for the generalized slab lens, then we would have generated one more arrangement that will exhibit the property of transferring images of sources in a perfect sense. If we define the new coordinates $q_1(x,y,z)$, $q_2(x,y,z)$, and $q_3(x,y,z)$ (assumed orthogonal), then in the new frame, the material parameters and fields are given by (Ward and Pendry 1996)

$$\tilde{\varepsilon}_i = \varepsilon_i \frac{Q_1 Q_2 Q_3}{Q_i^2}, \qquad \tilde{\mu}_i = \mu_i \frac{Q_1 Q_2 Q_3}{Q_i^2} \quad [35]$$

$$\tilde{E}_i = Q_i E_i, \qquad \tilde{H}_i = Q_i H_i \quad [36]$$

where

$$Q_i^2 = \left(\frac{\partial x}{\partial q_i}\right)^2 + \left(\frac{\partial y}{\partial q_i}\right)^2 + \left(\frac{\partial z}{\partial q_i}\right)^2 \quad [37]$$

Note that a distortion of space results in the change of ε and μ tensors in general. Thus, in many cases, the transformed geometry would involve spatially varying (inhomogeneous) and anisotropic medium parameters.

The change in geometry can also make it possible for us to realize lenses with curved surfaces. The original slab lens maps every point on the object plane to another point on the image plane. But the size of the image is identical to that of the source. This is due to the invariance in the transverse direction and the transverse wave vector (k_x, k_y) is preserved. In general, to change the size of the images, the translational symmetry would have to be broken and curved surfaces will necessarily be needed. The focussing action for the evanescent waves is crucially dependent on the near degeneracy of the surface plasmons in the case of the slab, and curved surfaces, in general, have a completely different dispersion for the surface plasmons. Thus, one should expect that inhomogeneous materials will be required for such curved lenses of negative refractive index. It can be shown (Ramakrishna 2005) that mapping the slab lens into cylindrical coordinates

$$x = r_0 e^{\ell/\ell_0} \cos\phi, \quad y = r_0 e^{\ell/\ell_0} \sin\phi, \quad z = Z \quad [38]$$

where ℓ_0 is some scale factor($=1$) generates a cylindrical annulus of inner and outer radii a_1 and a_2, respectively, with the material parameters given by

$$\begin{aligned} \varepsilon_r &= \mu_r = -1 \\ \varepsilon_\phi &= \mu_\phi = -1 \\ \varepsilon_z &= \mu_z = -1/r^2 \end{aligned} \quad [39]$$

for the annular region. The positive material outside the annular region should vary as

$$\begin{aligned} \varepsilon_r &= \mu_r = +1 \\ \varepsilon_\phi &= \mu_\phi = +1 \\ \varepsilon_z &= \mu_z = +1/r^2 \end{aligned} \quad [40]$$

where $r = r_0 \exp(\ell/\ell_0)$. This system transfers images in and out of the cylindrical annulus and the image of a source inside at $r = a_0$ will be formed on the surface $a_3 = a_0(a_2/a_1)^2$. Thus, there will be a magnification of the image by the factor

$$\mathcal{M} = \left(\frac{a_2}{a_1}\right)^2 \quad [41]$$

Note that these cylindrical lenses are also short-sighted in the same manner as the slab lens. They can only focus sources from inside to the outside only when $a_1^2/a_2 < r < a_1$, and the other way around from outside to the inner world when the source is located in $a_2 < r < a_2^2/a_1$.

Similarly the transformation into spherical coordinates $(r = r_0 e^{\ell/\ell_0}, \theta, \phi)$ can be used to generate a spherical perfect lens wherein a spherical shell of negative refractive material with $\varepsilon(r) \sim -1/r$ and $\mu(r) \sim -1/r$ with arbitrary dependence along θ and ϕ (which could be constant too!) have the property of perfectly transferring images of sources in and out of the shell (Pendry and Ramakrishna 2003). This spherical lens also has exactly the same magnification factor given by eqn [41]. In fact, the solutions in these two cases of a cylinder and sphere can also be obtained by a more conventional electromagnetic calculation in terms of the scattering modes (Ramakrishna 2005). One can obtain even more esoteric configurations such as one or two intersecting corners of negative refracting materials that behave as perfect lenses (Pendry and Ramakrishna 2003).

Other Approaches to Negative Refraction

There is also an approach to negative refractive materials based on loaded transmission lines (Eleftheriades *et al.* 2002), which has been implemented at radio- and microwave frequencies using lumped circuit elements. These show all the hallmarks of a negative refractive material within an effective medium approach.

Effects which can be interpreted as negative refraction have been observed in certain periodic photonic crystals (PCs) (Luo *et al.* 2003). An incident propagating plane wave from vacuum appears to undergo negative refraction inside the PC, and a slab of the PC can even work as a Veselago lens. The negative refraction in this case is a result of the curvature of the equifrequency surface and is present in spite of the right-handed nature of the propagation. In these instances, an effective permittivity and permeability cannot be easily ascribed to the crystal as the long wavelength condition is not met. It is difficult to homogenize the PC in the sense of meta-materials, and the energy transport in these PCs is very sensitive to the periodicity and the structural arrangements. Thus, it would be an over-simplification to characterize these effects in PC as merely due to an effective refractive index.

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Newtonian Fluids and Thermohydraulics

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Introduction

Thermohydraulics is based on the hypothesis of continuous medium. This hypothesis is easily satisfied since, for instance, a one-thousandth of 1 mm^3 of a perfect gas at normal temperature and pressure conditions (300 K, 1 atm) contains about 2.5×10^{13} molecules. Instantaneous balances are made inside a control volume fixed in the system of axes and crossed by the flows. The limit where this volume vanishes leads to the local formulation of the laws governing the flows. The flow is described by velocity $\vec{v}(\vec{r}, t)$, pressure $p(\vec{r}, t)$, temperature $T(\vec{r}, t)$, and other fields, $\vec{r}$ being the position vector of a point M, and t the time. The material derivative of $q(\vec{r}, t)$ is

$$\frac{Dq}{Dt} \equiv \left(\frac{\partial}{\partial t} + (\vec{v}\,.\,\vec{\nabla})\right) q$$

Let Q ($\vec{Q}$) be one of the scalar (vectorial) extensive quantities whose balance participates in the flow dynamics. It can be a quantity of matter, heat, impulse, or something else. Let ΔQ be the amount of Q contained in the volume $\Delta\mathcal{V}$ localized around M, and $q(\vec{r}, t)$ its local representative defined by

$$\rho(\vec{r}, t) q(\vec{r}, t) = \lim_{\Delta\mathcal{V} \to 0} \frac{\Delta Q}{\Delta\mathcal{V}} \equiv \frac{dQ}{d\mathcal{V}} \qquad [1]$$

where ρ is the density, similarly defined considering the case where $[Q]$ is taken as the mass m:

$$\rho(\vec{r}, t) = \frac{dm}{d\mathcal{V}} \qquad [2]$$

Table 1 gives examples of q quantities.

The instantaneous local balance of Q reads

$$\frac{\partial}{\partial t}(\rho q) + \vec{\nabla} \cdot \left(\vec{j}_Q + \rho q \vec{v}\right) = S_Q \qquad [3]$$

where S_Q stands for any possible local source of Q, and $\vec{j}_Q$ is the Q conduction flux density. **Figure 1** illustrates how these quantities allow us to evaluate the flux $d\Phi_Q = \vec{j}_Q \,.\, d\vec{S}$ of Q that instantaneously crosses a surface $d\vec{S}$. **Table 2** gathers the physical dimension of these notions for various Q's.

Table 1 Some quantities q. T is the absolute temperature, C_p the specific heat at constant pressure, and C the solute mass fraction

Mass	*Impulse*	*Kinetic energy*	*Heat*	*Mass fraction*
1	$\vec{v}$	$\frac{\vec{v}^2}{2}$	$C_p T$	$0 < C < 1$

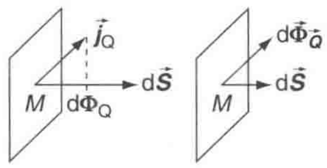


Figure 1 Q flux density and $\vec{Q}$ flux.

Table 2 Physical dimension of fluxes, flux densities, and $\vec{\nabla}\cdot$(flux density) for some q quantities

Q	*q*	*Flux*	*Flux density*	$\vec{\nabla}\cdot$*(flux density)*
Volume	undefined	m^{3}s^{-1}	[velocity]	s^{-1}
Mass	1	kgs^{-1}	kgs^{-1} m^{-2}	kgs^{-1} m^{-3}
Energy, heat	[velocity]^2	W	Wm^{-2}	Wm^{-3}
Electrical charge	Coulomb kg^{-1}	A	Am^{-2}	Am^{-3}
Impulse	[velocity]	[force]	[pressure]	[pressure] m^{-1}

For $\vec{Q}$, the flux densities are second-order tensors, since $d\vec{\Phi}_{\vec{Q}} = \vec{\vec{j}}_{\vec{Q}} \cdot d\vec{S}$ is vectorial (**Figure 1**). Its balance reads

$$\frac{\partial}{\partial t}(\rho\vec{q}) + \vec{\nabla} \cdot \left(\vec{\vec{j}}^{\,t}_{\vec{Q}} + \rho\vec{v} \otimes \vec{q}\right) = \vec{S}_{\vec{Q}} \qquad [4]$$

where ^{t} indicates the transposition and $\otimes$ a dyadic product. $\vec{j}_Q$ and $\vec{\vec{j}}_{\vec{Q}}$ are given later.

The governing equations of thermohydraulics are like [3] and [4]. They are completed by compatible initial and boundary conditions. The most general linear expression of the latter ones is of mixed type, for a scalar field,

$$\alpha q + \beta\left(\vec{\nabla} \cdot \hat{n}\right) q = \gamma \quad \text{on the boundary} \qquad [5]$$

α, β, and γ being prescribed data, and $\hat{n}$ the outward normal to the boundary. For a vectorial field, $\vec{q}$ and $\vec{\gamma}$, respectively, replace q and γ. The simplest cases are Dirichlet and Neumann boundary conditions with, respectively, $\beta = 0$ or $\alpha = 0$.

Governing Equations

We consider nonisothermal flows of fluids in thermodynamic conditions far from the critical point where acoustic effects are involved. The fluid is possibly a binary mixture, the simplest non-pure-fluid case where modeling does not raise conceptual difficulties. The

local composition is described by the solute (say) mass fraction,

$$C(M,t) = \lim_{\Delta V \to 0} \frac{\Delta m_{\text{solute}}}{\Delta m} = \frac{\rho_{\text{solute}}}{\rho}$$

with $0 \le C \le 1$. Only thermodiffusion is treated, and the influence the solutal gradient has on the heat flux is not considered, being negligible in liquid mixtures. The coupling between the heat and species molecular transports then comes only in the solutal flux density relation

$$\vec{j}_{\text{solute}} = -\rho\kappa_C(T,C)\left[\vec{\nabla}C + C(1-C)S_T\vec{\nabla}T\right] \quad [6]$$

with $\kappa_C > 0$, and $S_T(T,C)$, the solute Soret coefficient, which is positive or negative. The order of magnitude of the Soret coefficient in the molecular solutions does not exceed few $10^{-2}\,\text{K}^{-1}$, while for colloidal solutions (ferrofluids) $|S_T|$ can be in the range 0.03–$0.5\,\text{K}^{-1}$. Even if small, the induced mass fraction separation, $\Delta C \simeq S_T\Delta T$, generates a solutal buoyancy of significant dynamical influence.

Equation of State for the Density

One must first describe the sensitivity of the density, $\rho(p,T,C)$, upon pressure, temperature, and mass fraction in static conditions. The pressure and temperature effective ranges, Δp and ΔT, are assumed small enough compared to their respective mean values, p_0 and T_0, for the local (at $\rho_0 \equiv \rho(p_0,T_0,C_0)$) tangent to $\rho(p,T,C)$ to be a good approximation in most cases,

$$\frac{\rho-\rho_0}{\rho_0} = \chi(p-p_0) - \alpha_T(T-T_0) + \alpha_C(C-C_0) \quad [7]$$

where

$$\chi = \frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial p}\right)\bigg|_0$$

and

$$\alpha_T = -\frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial T}\right)\bigg|_0, \qquad \alpha_C = \frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial C}\right)\bigg|_0$$

are the compressibility, thermal, and solutal expansion positive coefficients, and C_0 is the solute mean mass fraction. Thermodynamic properties of some fluids are given in **Table 3**. Equation [7] is valid if $\chi\Delta p$, $\alpha_T\Delta T$, and $\alpha_C|\Delta C|$ are $\ll 1$. Moreover, in laboratory experiments and industrial processes, one generally has $\Delta p/p_0 \ll \Delta T/T_0$. The pressure term in [7] can thus be neglected in thermohydraulics.

Table 3 Some values of density, thermal expansion and compressibility coefficients, specific heat at constant pressure, and sound speed at $p = 1$ atm and $T = 293$ K; in SI units

Fluid	ρ	αT	χp	C_p	c
Air	1.205	1	1	1005	344
Helium	0.167	1	1	5227	1010
CO_2	1.841	1	1	832	269
Water	1000	0.0607	4.91×10^{-5}	4182	1461
Glycerol	1250	0.148	2.2×10^{-6}	2333	2044
Mercury	13579	0.0533	3.76×10^{-6}	1391	1409

Notice that water density exhibits a maximum around 4°C. A quadratic term in T must then be added to [7].

The Boussinesq Approximations

The parameter $\alpha_T\Delta T \ll 1$ is the primary source of thermohydraulics. Therefore, the $\vec{v}, p, T$ and C fields can be expanded in series of terms of increasing power in $\alpha_T\Delta T$. The leading term of each series contains an important part of the interesting dynamics. The forthcoming equations are given in the corresponding approximation framework. They contain many simplifications, due to Boussinesq. For instance, the conductivities and diffusivities are taken as constant, as well as $C(1-C)S_T$ in eqn [6]. The next approximation step, the low-Mach model, keeps the leading compressibility and expansion effects, while discarding the associated acoustic waves. This gives access to thermo-soluto-acoustic phenomena. Expansion oscillations are indeed able to trigger, and sustain, acoustic waves provided phase agreements are fulfilled. This second-order model is not presented here.

The compliance with the criteria $\alpha_T\Delta T \ll 1$ and $\alpha_C|\Delta C| \ll 1$ must be checked case by case. The section "Steady parallel-flow model" briefly illustrates this point with an example of thermally driven flow. Furthermore, the T- and C-sensitivity of S_T is an experimental fact that requires a generic approach of the problem. The C-sensitivity of the physical properties is generally more pronounced, nonmonotonic, for instance, over $C \in [0,1]$, than their T-sensitivity.

Boussinesq Local Balances

Mass It reads $\partial\rho/\partial t + \vec{\nabla}\cdot(\rho\vec{v}) = 0$, or equivalently $(1/\rho)(D\rho/Dt) = -\vec{\nabla}\cdot\vec{v}$. The fluid particle density varies along its trajectory by compressibility and thermo-solutal expansion. At the leading order in $\alpha_T\Delta T$ and $\alpha_C|\Delta C|$, the latter is negligible, whereas the former is associated with acoustics effects, also negligible when the fluid velocity is much smaller

than the sound speed. The mass balance equation then reduces to

$$\vec{\nabla} \cdot \vec{v} = 0 \qquad [8]$$

Only transverse velocity waves (or shear waves) are allowed by this equation, $\vec{v} \simeq e^{i(\vec{k}\cdot\vec{r}+\omega t)}$ with $\vec{k} \cdot \vec{v} = 0$, since acoustics contributions are discarded.

Impulse The impulse molecular flux density is

$$\vec{\vec{j}}_{\rho\vec{v}} = p\,\vec{\vec{1}} - \mu_{\vec{v}}\left[\vec{\nabla} \otimes \vec{v} + (\vec{\nabla} \otimes \vec{v})^t\right]$$

where $\mu_{\vec{v}}$ is the impulse conductivity and $\vec{\vec{1}}$ the Kronecker tensor. A Newtonian fluid is defined as having $\mu_{\vec{v}}$ constant with respect to the rate-of-strain tensor $\vec{\nabla} \otimes \vec{v}$. The impulse balance then reads

$$\frac{\partial}{\partial t}(\rho\vec{v}) + \vec{\nabla} \cdot (\rho\vec{v} \otimes \vec{v}) + \vec{\nabla} \cdot \vec{\vec{j}}_{\rho\vec{v}} = \rho\vec{\Gamma}$$

In the source term $\rho\vec{\Gamma}$, $\vec{\Gamma} = \vec{g}$ for gravity-driven buoyant flows.

With the aforementioned approximations, the impulse balance becomes

$$\frac{D\vec{v}}{Dt} = -\frac{1}{\rho_0}\vec{\nabla}P + \frac{\rho - \rho_0}{\rho_0}\vec{g} + \nu\vec{\nabla}^2\vec{v} \qquad [9]$$

with

$$\frac{\rho - \rho_0}{\rho_0} = -\alpha_T(T - T_0) + \alpha_C(C - C_0)$$

$$\nu = \frac{\mu_{\vec{v}}}{\rho_0}$$

the impulse diffusivity, and the pressure $P = p - p_{0,h}$, $p_{0,h}$ satisfying the hydrostatic relation

$$\vec{\nabla}p_{0,h} = \rho_0\vec{g}$$

In the rotating frame of vector $\vec{\Omega}(t)$,

$$\frac{\rho - \rho_0}{\rho_0}\vec{\Omega} \wedge (\vec{\Omega} \wedge \vec{r}) + 2\vec{\Omega} \wedge \vec{v} + \frac{d\vec{\Omega}}{dt} \wedge \vec{r}$$

must be subtracted from the right-hand side of [9] and $p_{0,h}$ redefined by

$$\vec{\nabla}p_{0,h} = \rho_0\left(\vec{g} - \vec{\Omega} \wedge (\vec{\Omega} \wedge \vec{r})\right)$$

On a free surface, a particular velocity boundary condition is to be established. Let $d\vec{S} = dS\,\hat{n}$ be a surface element located around M. The tangential component ($\hat{t} \cdot \hat{n} = 0$) of the impulse flux across $d\vec{S}$,

$$\hat{t} \cdot d\vec{f} = \hat{t} \cdot \vec{\vec{j}}_{\rho\vec{v}} \cdot d\vec{S} = -\mu_{\vec{v}}\hat{t} \cdot \left[\vec{\nabla} \otimes \vec{v} + (\vec{\nabla} \otimes \vec{v})^t\right] \cdot d\vec{S}$$

must be continuous. Surface tension $\sigma(T, C)$ inhomogeneities make the free surface a source of impulse which diffuses in the fluid core. A flow occurs even with $\vec{\Gamma} = 0$. For the fluid located where $d\vec{S}$ points to, the velocity boundary condition on the free surface then reads

$$-\mu_{\vec{v}}\hat{t} \cdot \left[\vec{\nabla} \otimes \vec{v} + (\vec{\nabla} \otimes \vec{v})^t\right] \cdot \hat{n} = (\vec{\nabla} \cdot \hat{t})\sigma \qquad [10]$$

with

$$(\vec{\nabla} \cdot \hat{t})\sigma = \frac{\partial\sigma}{\partial T}(\vec{\nabla} \cdot \hat{t})T + \frac{\partial\sigma}{\partial C}(\vec{\nabla} \cdot \hat{t})C$$

For most fluids, $\partial\sigma/\partial T < 0$. In the Boussinesq framework $\partial\sigma/\partial T$ and $\partial\sigma/\partial C$ are constant. Equation [10] couples the impulse balance with the heat and composition ones.

Heat Local thermodynamic equilibrium is assumed. The molecular heat flux density is $\vec{j}_{\text{heat}} = -\mu_T\vec{\nabla}T$, with μ_T the thermal conductivity. The approximate heat balance reads

$$\frac{DT}{Dt} = \kappa_T\vec{\nabla}^2 T + S_{\text{heat}} \qquad [11]$$

where $\kappa_T = \mu_T/(\rho_0 C_p)$ is the heat diffusivity and S_{heat} a possible local (Joule, radioactive,…) heat source. Thermohydraulics can simply be driven by nonuniform thermal conditions imposed along the fluid boundary, and in this article we henceforth take $S_{\text{heat}} = 0$.

Mass fraction Approximating [6] yields the mass fraction balance,

$$\frac{DC}{Dt} = \kappa_C\vec{\nabla}^2 C + C_0(1 - C_0)S_T\vec{\nabla}^2 T \qquad [12]$$

where κ_C and S_T are evaluated at T_0 and C_0. The normal flux condition

$$\left(\vec{\nabla}C \cdot \hat{n}\right) = -C_0(1 - C_0)S_T\left(\vec{\nabla}T \cdot \hat{n}\right)$$

is imposed on impervious boundaries.

The Hydrostatic State

Knowing whether the fluid can be in static state with respect to its presupposed rigid container helps for a first understanding of thermohydraulic dynamics. This raises two problems: (1) the existence of this state and (2) its stability, discussed

later. Point (1) requires the fulfilment of three relations,

$$\vec{\nabla}p = \rho(p, T, C)\vec{\Gamma} \quad [13]$$

$$\begin{aligned} \frac{\partial T}{\partial t} &= \kappa_T \vec{\nabla}^2 T \\ \frac{\partial C}{\partial t} &= \kappa_C \vec{\nabla}^2 C + C_0(1 - C_0) S_T \vec{\nabla}^2 T \end{aligned} \quad [14]$$

The curl of [13] yields

$$\vec{\nabla}\rho(p, T, C) \wedge \vec{\Gamma} + \rho(p, T, C)\vec{\nabla} \wedge \vec{\Gamma} = 0$$

which has no reason to be generically satisfied since $\rho(p, T, C)$ and $\vec{\Gamma}$ are totally uncorrelated. The hydrostatic state cannot exist if $\vec{\Gamma}$ does not derive from a scalar potential, as with

$$\vec{\Gamma} = \vec{g} - \vec{\Omega} \wedge (\vec{\Omega} \wedge \vec{r}) - \frac{d\vec{\Omega}}{dt} \wedge \vec{r} \quad \text{if } \frac{d\vec{\Omega}}{dt} \neq 0$$

The Earth's rotation axis is known to precess with a period of about 26 000 years. This generates a component of 26 000 years timescale in the atmospheric, oceanic, and internal flows.

Considering now that

$$\vec{\Gamma} = -\vec{\nabla}\psi$$

the existence of a hydrostatic state only depends on the simultaneous verification of [14] and

$$\vec{\nabla}\rho(p, T, C) \wedge \vec{\nabla}\psi = 0 \quad [15]$$

Iso-ψ surfaces must therefore coincide with isopycnal, isobaric, iso-T, and iso-C surfaces since the p, T, and C sensitivities of ρ are uncorrelated. The compatibility of this condition with [14] is the key for concluding about the existence of the hydrostatic state. Considering again our planet as an example (forgetting about precession), the iso-ψ surfaces are almost ellipsoidal. Such T and C distributions cannot satisfy [14]. Thus, the atmospheric and oceanic dynamics, and thermohydraulics as well, are due to a nonvanishing thermal torque, $\vec{\nabla}T \wedge \vec{\nabla}\psi$.

A free surface in hydrostatic state is isothermal and isocompositional, by eqn [10], whatever $\vec{\Gamma}$.

Dimensionless Local Balances

In buoyancy-driven thermohydraulics, we consider four velocity scales – three of molecular origin, and the fourth is the free-fall velocity in the buoyancy,

Table 4 Orders of magnitude of the Prandtl number for the usual fluids. Air and water are in normal conditions

Liquid metals	Gases	Water	Oils
Several 10^{-3} – 10^{-2}	$\simeq 1$, 0.7 for air	6.7	>10

$$V_1 = \frac{\kappa_T}{L}, \quad V_2 = \frac{\kappa_C}{L}, \quad V_3 = \frac{\nu}{L}$$
$$V_4 = \sqrt{\alpha_T \Delta T g L}$$

L being a fluid container size scale. Thence come the Rayleigh, Prandtl and Lewis numbers,

$$Ra = \frac{V_4^2}{V_1 V_3} = \alpha_T \Delta T \frac{gL^3}{\nu \kappa_T}$$
$$Pr = \frac{V_3}{V_1} = \frac{\nu}{\kappa_T}, \qquad Le = \frac{V_2}{V_1} = \frac{\kappa_C}{\kappa_T}$$

Ra being the experimental control parameter, and $Le \ll 1$. **Table 4** gives Pr orders of magnitude for usual fluids. Let V be the fluid velocity amplitude. The importance of the thermal, solutal, and impulse convections with respect to the corresponding diffusions is, respectively, estimated by the thermal, compositional Péclet and Reynolds numbers,

$$Pe_T = \frac{V}{V_1} = \frac{VL}{\kappa_T}, \qquad Pe_C = \frac{V}{V_2} = \frac{VL}{\kappa_C}$$
$$Re = \frac{V}{V_3} = \frac{VL}{\nu}$$

with

$$Pr = \frac{Pe_T}{Re}, \quad Le = \frac{Pe_C}{Re}, \qquad Ra = (Pe_T Re)_{|V=V_4}$$

Capillary thermohydraulics introduces one velocity scale and the Marangoni number,

$$V_5 = \frac{|\Delta\sigma|}{\mu_{\vec{v}}}, \qquad Ma = \frac{V_5}{V_1} = Pe_T$$

with $\Delta\sigma = (d\sigma/dT)\Delta T$ in pure fluid. A small capillary number, $Ca = |\Delta\sigma|/\sigma$, indicates a weak influence of the dynamics upon the free-surface curvature.

Let V_1, $\Pi = \rho_0 V_1^2$, $\tau = L/V_1$, ΔT and

$$\Delta C = -C_0(1 - C_0) S_T \Delta T$$

be the velocity, pressure, time, temperature, and mass fraction scales, with

$$\Theta = \frac{T - T_0}{\Delta T} \quad \text{and} \quad \mathcal{C} = \frac{C - C_0}{\Delta C}$$

the reduced temperature and mass fraction, respectively. The other quantities, coordinates included, are similarly reduced and noted identically.

Equation [8] does not change and [9], [11] and [12] become, respectively,

$$\frac{D\vec{v}}{Dt} = -\vec{\nabla}P + Pr\left[Ra(\Theta + \Psi_B C)\hat{e}_z + \vec{\nabla}^2\vec{v}\right] \quad [16]$$

$$\frac{D\Theta}{Dt} = \vec{\nabla}^2\Theta \quad [17]$$

$$\frac{DC}{Dt} = Le\vec{\nabla}^2 C - \vec{\nabla}^2\Theta \quad [18]$$

where

$$\Psi_B = -\frac{\alpha_C \Delta C}{\alpha_T \Delta T}$$

is the buoyancy separation ratio and $\hat{e}_z = -\vec{g}/|\vec{g}|$. A $\Psi_B < 0$ (>0) corresponds to opposite (cooperative) thermal and solutal buoyancies. The reduced mass fraction boundary condition on impervious walls is

$$\left(\vec{\nabla}C \cdot \hat{n}\right) = \left(\vec{\nabla}\Theta \cdot \hat{n}\right) \quad [19]$$

In rotating frame, scaling $\vec{\Omega}(t)$ by Ω_0, $\bar{\vec{\Omega}}(t) = \vec{\Omega}(t)/\Omega_0$,

$$Ra\, Fr\,(\Theta + \Psi_B C)\bar{\vec{\Omega}} \wedge (\bar{\vec{\Omega}} \wedge \vec{r}) - \frac{1}{Ek}\left(2\bar{\vec{\Omega}} \wedge \vec{v} + \frac{d\bar{\vec{\Omega}}}{dt} \wedge \vec{r}\right)$$

must be added inside the square-bracket term of [16]. The Froude and Ekman numbers appear as

$$Fr = \frac{\Omega_0^2 L}{g}, \qquad Ek = \frac{\nu}{\Omega_0 L^2}$$

The dimensionless capillarity stress condition [10] reads

$$\hat{t} \cdot \left[\vec{\nabla} \otimes \vec{v} + (\vec{\nabla} \otimes \vec{v})^t\right] \cdot \hat{n} = -Ma\left((\vec{\nabla} \cdot \hat{t})\Theta + \Psi_C(\vec{\nabla} \cdot \hat{t})\,C\right) \quad [20]$$

with

$$\Psi_C = \frac{\partial\sigma/\partial C}{\partial\sigma/\partial T}\frac{\Delta C}{\Delta T}$$

the capillarity separation ratio, and

$$Ma = \left|\frac{\partial\sigma}{\partial T}\frac{\Delta T}{\mu_{\vec{v}} V_1}\right|$$

These equations show that, in the Boussinesq framework, the flow physics does not depend on p_0, T_0, and C_0, except through the material properties which enter the numbers.

Linear Stability

Given a base state $\mathcal{S} = (\vec{v}, \Theta, C)$, a solution of [8], [16]–[18], how does it behave in presence of an infinitesimal disturbance $(\delta\vec{v}, \delta\Theta, \delta C)$? Applying [8], [16]–[18] to $(\vec{v} + \delta\vec{v}, \Theta + \delta\Theta, C + \delta C)$ and discarding the quadratic terms in perturbation provide the disturbance temporal evolution,

$$\vec{\nabla} . (\delta\vec{v}) = 0 \quad [21]$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\delta\vec{v}\\ \delta\Theta\\ \delta C\end{pmatrix} = \mathcal{F} + \left(\delta\vec{v} \cdot \vec{\nabla}\right)\begin{pmatrix}\vec{v}\\ \Theta\\ C\end{pmatrix} + \mathcal{A}\begin{pmatrix}\delta\vec{v}\\ \delta\Theta\\ \delta C\end{pmatrix} \quad [22]$$

where $\mathcal{F} = (-\vec{\nabla}(\delta P), 0, 0)^t$, and

$$\mathcal{A} = \begin{pmatrix}\mathcal{B}_{Pr} & Ra\,Pr\,\hat{e}_z & Ra\,Pr\,\Psi_B\,\hat{e}_z\\ 0 & \mathcal{B}_1 & 0\\ 0 & -\vec{\nabla}^2 & \mathcal{B}_{Le}\end{pmatrix} \quad [23]$$

with $\mathcal{B}_a = -(\vec{v} \cdot \vec{\nabla}) + a\vec{\nabla}^2$. The perturbations ($\delta\vec{v}$, $\delta\Theta$, δC) have the $(\vec{v}, \Theta, C)$ boundary conditions, but homogeneous. On a free surface, the perturbation capillary stress condition is

$$\hat{t} \cdot \left[\vec{\nabla} \otimes \delta\vec{v} + (\vec{\nabla} \otimes \delta\vec{v})^t\right] \cdot \hat{n} = -Ma\left((\vec{\nabla} \cdot \hat{t})\delta\Theta + \Psi_C(\vec{\nabla} \cdot \hat{t})\delta C\right) \quad [24]$$

Recasting [21]–[23] provides

$$\frac{\partial}{\partial t}\begin{pmatrix}\delta\vec{v}\\ \delta\Theta\\ \delta C\end{pmatrix} = \mathcal{L}(\mathcal{S})\begin{pmatrix}\delta\vec{v}\\ \delta\Theta\\ \delta C\end{pmatrix} \quad [25]$$

whose solution is

$$\begin{pmatrix}\delta\vec{v}(t)\\ \delta\Theta(t)\\ \delta C(t)\end{pmatrix} = e^{\mathcal{L}(\mathcal{S})t}\begin{pmatrix}\delta\vec{v}(t=0)\\ \delta\Theta(t=0)\\ \delta C(t=0)\end{pmatrix} \quad [26]$$

Direct System

$\mathcal{L}(\mathcal{S})$ is made of $\vec{\nabla}$ acting on the initial perturbation. Conclusions about $\mathcal{S}$ stability depend on the sign of λ_{max}, the real part of the leading eigenvalue of $\mathcal{L}$ found with all the possible perturbations. There is stability if $\lambda_{max} < 0$. At $\lambda_{max} = 0$, the marginal stability, the bifurcation threshold is located at $Ra\,(Pr, Le, \Psi_B, \Psi_C, X) = Ra_c$, Ra_c-being the critical value of the control parameter, X containing all the other parameters of the problem (container aspect ratios, etc.). The nonlinear-stability analysis in the vicinity of Ra_c supplies ξ in $\lambda_{max} \propto (Ra - Ra_c)^\xi$, which is characteristic of the bifurcation.

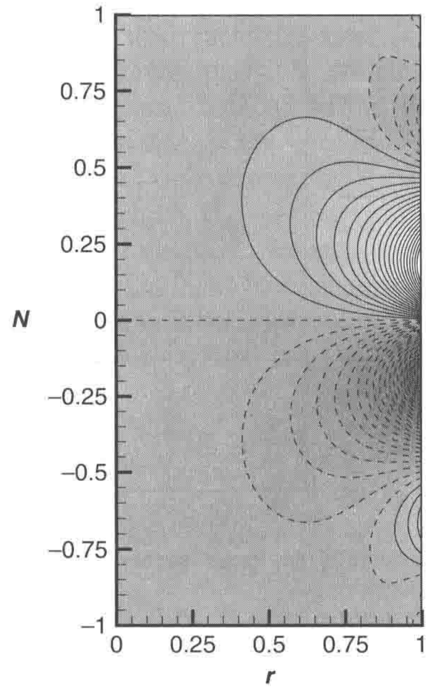


Figure 2 Leading axisymmetric thermal adjoint eigenvector (Courtesy of O Bouizi and C Delcarte).

Adjoint System

The leading left eigenmode complex conjugate supplies the response field of the base state to the most destabilizing punctual disturbances.

The $\mathcal{S}$ state and $\mathcal{L}$ eigenspace analytical determinations are often impossible. One must resort to specifically designed numerical tools. A numerical adjoint eigenvector is presented in **Figure 2** for a ($Ma = 106$, $Pr = 10^{-2}$) side-heated cylindrical liquid bridge, with a free surface on the right and the axis on the left.

Nonlinear Stability

When $\lambda_{\max} > 0$, the associated disturbance exponentially grows with time, until nonlinearities become essential. The flow progressively evolves from $\mathcal{S}$ towards a new state, $\mathcal{S}'$, which is a solution of [8], [16]–[18]. How can one proceed analytically to know how the nonlinearities control the bifurcation? A large number of $\mathcal{S} \rightarrow \mathcal{S}'$ bifurcations exist, with either both $\mathcal{S}, \mathcal{S}'$, steady or unsteady but with different flow structure, or one is steady and the other is not. Bifurcations can also be reversible or hysteretic, with respect to Ra. The symmetries of $\mathcal{S}$ play an important role and non-Boussinesq effects change the thresholds and the nature of bifurcation.

Landau's works have opened up the way to the theory of nonlinear hydrodynamic stability. The ruling equations are reduced, using an appropriate expansion method, to a set of ordinary differential equations describing the temporal evolution of amplitudes, A_i, $i = 1, 2, \ldots, I$, characterizing the perturbation eigenmodes,

$$\frac{\mathrm{d}A_i}{\mathrm{d}t} = \lambda_i A_i + N_i(A_j) \quad \text{for } i, j = 1, 2, \ldots, I \qquad [27]$$

where N accounts for the nonlinear action of the I modes on A_i, and the λ_i's are the temporal growth rates coming from the linear theory. The stability of the steady solutions, $\mathrm{d}A_i/\mathrm{d}t = 0$, is determined by local analysis. With one destabilizing mode, the simplest model is $\mathrm{d}A/\mathrm{d}t = \lambda A - \alpha A|A|$, with $\alpha > 0$, constant, specific of the bifurcation. Symmetry considerations (some of them directly originate from the Boussinesq framework) may impose $\alpha = 0$, whereby the simplest model becomes $\mathrm{d}A/\mathrm{d}t = \lambda A + \beta A^3$, with β another constant.

When the flow is weakly confined in one or two space directions, boundary effects can play a subtle dynamical role, allowing, for instance, the existence of multiple solutions, each one made of many interacting modes. A large variety of flow regimes is then observed, as steady/traveling, extended/localized wave packets, particularly in binary mixtures. Spacetime models, close to [27], such as the Ginzburg–Landau equation,

$$\frac{\partial A}{\partial t} = \lambda A + \alpha \frac{\partial^2 A}{\partial x^2} + \beta |A|^2 A$$

are derived for describing the dynamics of the wave packet envelop (of complex amplitude A).

Hydrostatic State Stability

The static-state stability is analytically tractable in unbounded volume. Transverse wave (by [21]) solutions are the potentially destabilizing perturbations, with wave vector $\vec{k}$ and complex frequency ω. The system [22]–[23] gets simplified, and $\mathcal{L}$ becomes algebraic upon substituting $(\mathrm{i}\vec{k}, \mathrm{i}\omega)$ for $(\vec{\nabla}, \partial/\partial t)$. Intuitively, the quiescent state loses its stability when $\vec{\nabla}\rho(p, T, C) \cdot \vec{\nabla}\psi$ exceeds a threshold value (positive, by the dissipative effects). This analysis supplies it, together with the data of the oscillatory motions emerging at onset from the rest-state instability.

In reality, the fluid is confined to three dimensions, possibly with free surfaces, and wave solutions are no longer usable. The first approach consists in defining a simplified model confined to one dimension. The perturbations must satisfy homogeneous boundary conditions, and/or [24], and they are waves in both other space directions. The resulting problem may be analytically tractable. The stability of many quiescent-state configurations was studied, for fluid layers of infinite or very large

extension, of pure-fluid/mixtures, with/without free surface. Nonetheless, many other configurations are not yet analyzed. Two- and three-dimensional cases must be numerically treated.

Gravitational Buoyancy Convection

Among the numberless thermal situations to analyze, research mainly favored the case where the fluid is confined in simple geometries and submitted to two distinct heating directions, $\vec{\nabla}T$ being either aligned or normal to $\vec{\Gamma}$, that is vertical or horizontal in the gravity field. Each case leads to specific thermohydraulics. The rest-state stability is the first analysis step of the former case, the first to be experimentally studied by Bénard in 1900, with a horizontal liquid layer. The latter is of more recent interest, with Batchelor's theoretical work on the parallel convective regimes of pure fluid confined in tall slot. Since then, a large amount of work has been published on those cases, tackling various confinement geometries, and involving high Ra values. This problem became the paradigm of the rich spatiotemporal behaviors arising in nonlinear systems driven away from equilibrium. In binary mixtures the complexity of the dynamics increases considerably. The literature is so far practically devoid of any three-dimensional results in mixtures. Ternary mixtures have so far been only scarcely considered.

Steady Parallel-Flow Model

This analytical approach comes from an interesting Batchelor's remark made about the vorticity but here applied to the velocity of a confined flow. "A number of flow fields are characterized by values of the magnitude of the" velocity "in the neighborhood of a certain line in the fluid which are much larger than those elsewhere," and (by $\vec{\nabla}\cdot\vec{v}=0$) "this line of necessity" is parallel to $\vec{v}$ and to the container walls.

Buoyant forces may contradict this assertion, particularly in Rayleigh–Bénard configuration with imposed temperatures. There, no parallel solution exists. Nevertheless, steady parallel flows do exist in containers. The thermally active walls (whatever they be – the largest or smallest) are either maintained at constant temperatures, or subjected to a constant heat flux. **Figure 3** sketches a cross section (hereafter referred to as the vertical midplane) of such a configuration, with active (uniform heating q) vertical walls. The other sides are adiabatic. No rest state is allowed here. Although intrinsically three dimensional, the steady regime in

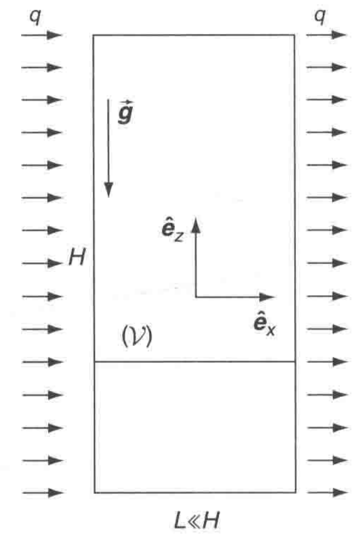


Figure 3 Sketch of the cross section of a slender vertical container.

this cavity can be fairly well approximated as two dimensional (in the vertical midplane), and moreover mainly parallel to the active walls, in an Ra range which increases with the aspect ratio, H/L. The influence of the horizontal sides is of limited range compared to the flow extension, H. The parallel flow is then the one-dimensional approximation of what occurs in the major part of the cavity. This configuration is taken with a binary mixture for illustrating an approach applicable with minor variations in other situations.

The problem becomes linear. Indeed, $\vec{v}=w(x)\hat{e}_z$ by $\vec{\nabla}\cdot\vec{v}=0$. Taking $\Delta T=qL/\mu_T$ as temperature scale, [16]–[18] imply

$$\Theta(x,z)=G_T z+\hat{\Theta}(x), \qquad \mathcal{C}(x,z)=G_C z+\hat{\mathcal{C}}(x)$$

with G_T, G_C as constants. The impulse balance is

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2}=-Ra\left[\hat{\Theta}(x)+\Psi_B\hat{\mathcal{C}}(x)\right] \qquad [28]$$

and the ruling equations

$$\frac{\mathrm{d}^4 w}{\mathrm{d}x^4}=-Ra\left[G_T+\frac{\Psi_B}{Le}(G_T+G_C)\right]w$$
$$wG_T=\frac{\mathrm{d}^2\hat{\Theta}}{\mathrm{d}x^2}, \qquad w(G_T+G_C)=Le\frac{\mathrm{d}^2\hat{\mathcal{C}}}{\mathrm{d}x^2} \qquad [29]$$

An internal length scale is predicted, of thickness

$$\left[Ra\left(G_T+\frac{\Psi_B}{Le}(G_T+G_C)\right)\right]^{-1/4}$$

By [28] and [19], the thermal flux condition yields

$$\left.\frac{\mathrm{d}^3 w}{\mathrm{d}x^3}\right|_{x=\pm 1/2}=-Ra\,(1+\Psi_B)$$

A last operation allows to determine G_T and G_C. The overall heat and mass fraction balances are performed in the cavity part $(\mathcal{V})$, which is bounded by an horizontal plane located within the parallel-flow region. Since the walls are impervious, the solute is transported only across the lower boundary of $(\mathcal{V})$, through which the net vertical convective supply must be balanced, in steady regime, by vertical diffusion. The heat balance works similarly, since the walls are adiabatic or submitted to equal fluxes. Whence the relations,

$$\int_{-1/2}^{1/2} w(x)\hat{\Theta}(x)\,\mathrm{d}x = G_T$$

$$\int_{-1/2}^{1/2} w(x)\hat{C}(x)\,\mathrm{d}x = G_T + G_C$$

The steady parallel flow is determined. Its stability can be analyzed as indicated in the section "Linear stability."

Some caution must be taken for the Boussinesq approximations to be valid here, with the temperature and mass fraction increasing constantly (by G_T, G_C) along the direction of largest cavity extension. These gradients are at the origin of the "thermogravitational column" separation power, a device designed for the isotope separation. Extremely long columns can provide almost complete separations, with $\alpha_C|\Delta C|$ no longer $\ll 1$, and then the non-Boussinesq effects occur.

As an illustration of aforementioned notions, let us consider the $(Pr=1,\ Le=0.1)$ Rayleigh–Bénard–Soret (RBS) problem where horizontal solid plates of infinite extension are uniformly heated from above $(Ra < 0)$ or below $(Ra > 0)$. This configuration is simply obtained by rotating the cavity in **Figure 3** by $\pm\pi/2$ with respect to $\vec{g}$ and to $(\hat{e}_x, \hat{e}_z)$. The steady parallel-flow model can lead to the right-hand side of an equation like [27] governing the time evolution of A, the parallel-flow amplitude,

$$\frac{\mathrm{d}A}{\mathrm{d}t} \propto A\left[\mathrm{Le}^{-2}A^4 + \alpha\left(1 + \frac{1-r}{Le^2}\right)A^2 + \alpha^2\left(1 - \frac{r}{r_c}\right)\right] \qquad [30]$$

where

$$\alpha = \frac{315}{218}, \quad r = \frac{Ra}{720}, \quad r_c = \left[1 + \Psi_B(1 + Le^{-1})\right]^{-1}$$

Here r_c is the critical value or r where the rest state loses its stability towards a steady parallel flow. The roots of $\mathrm{d}A/\mathrm{d}t = 0$ are $A = A_0 = 0, A = A_{\|}(r, Le, \Psi_B)$, for the quiescent, convective states. **Figure 4** shows that $A_0 = 0$ and the curves $A_{\|}(r)$ for several

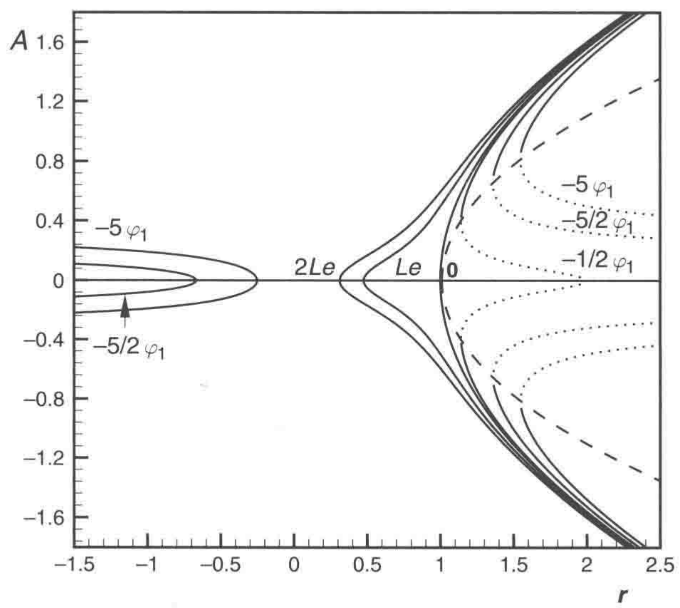


Figure 4 Bifurcation diagram of $A_0(r)$ and $A_{\|}(r)$ for various separation ratios $\Psi_B(Le)$.

$\Psi_B(Le)$, $\varphi_1 = -(1 + Le^{-1})^{-1}$ being the r_c pole. The solid (dotted) parts correspond to the stable (unstable) steady states, emerging from direct (backward) pitchfork bifurcations of the rest state at r_c. Saddle–node bifurcations from unstable to stable steady states are also predicted, on the dashed curve of the equation

$$\widehat{A_{\|}}(r) = \pm\sqrt{\frac{\alpha}{2}}\sqrt{r - (1 + Le^2)}$$

Fully Nonlinear Problem

Numerical tools are required for solving the system [8], [16]–[18] and analyzing the stability of the flows obtained.

The RBS Case Let us illustrate how the rest-state loss of stability occurs in the two-dimensional RBS case, with a $(Pr=1,\ Le=0.1,\ \Psi_B=-0.2)$ mixture. The flow lies in the meridian plane of an axisymmetric container with the radius/height ratio equal to 2. No-slip conditions are imposed on impervious walls; the temperature on the bottom plate is higher than on top, and the peripheral wall is adiabatic. At $t=0$, the quiescent state is given a small random perturbation. The system evolves (**Figure 5**) towards a stable periodic solution via a transient regime of exponentially amplified amplitude (eqn [26]). One speaks of a Hopf bifurcation for a steady (here quiescent) state destabilization by oscillatory disturbances.

The "instantaneous" frequency (from the time running between two successive identical passes of

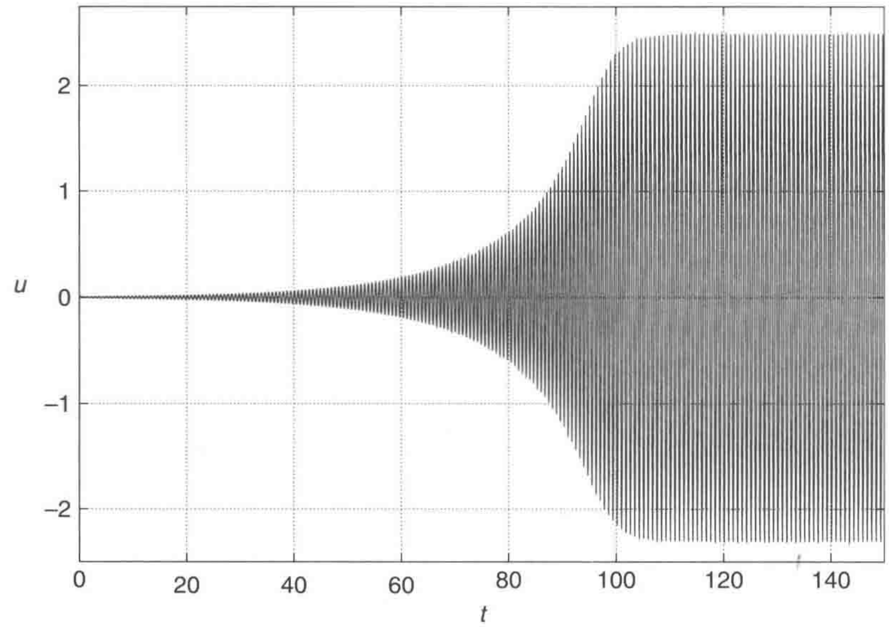


Figure 5 Time evolution of a radial velocity nodal value for $Ra = 2600$. Reproduced from Millour, Labrosse, and Tric (2003) *Physics of Fluids* 15(10): 2791–2802, with permission from American Institute of Physics.

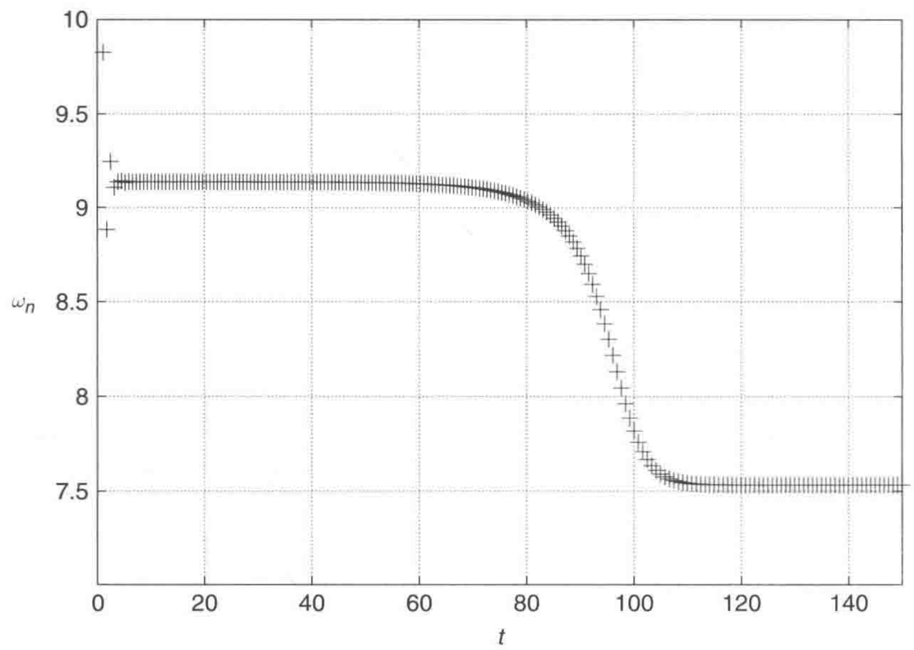


Figure 6 Instantaneous angular frequency ω_n corresponding to **Figure 5**. Reproduced from Millour, Labrosse, and Tric (2003) *Physics of Fluids* 15(10): 2791–2802, with permission from American Institute of Physics.

the signal) evolves with time (**Figure 6**) from its threshold value to its nonlinearly saturated one.

Accurate determination the thresholds and identification of the associated bifurcation is possible by fitting the argument ξ of $\lambda_{\max}(Ra)$ from the exponential growth of **Figure 5**, in the Ra_c vicinity. **Figure 7** shows (solid dots) $\lambda(Ra)$ measurements, and the solid line (in **Figure 8** also) is the linear law given by the two points closest to the vanishing growth rate. The local law announced in the subsection "Direct system" is confirmed, with an exponent $\xi = 1$ for the Hopf bifurcation, and $\xi = 1/2$ for saddle–node (**Figure 8**) and pitchfork bifurcations.

The Thermally Driven Cubic Cavity All flows are obviously three dimensional. When do they possess a two-dimensional approximation? How to qualify it? Clearly, the flow that develops in the container of **Figure 3** might enjoy (in a given parameter domain, $\mathcal{D}$) the mirror-reflection symmetry property about the vertical midplane. Is there a two-dimensional

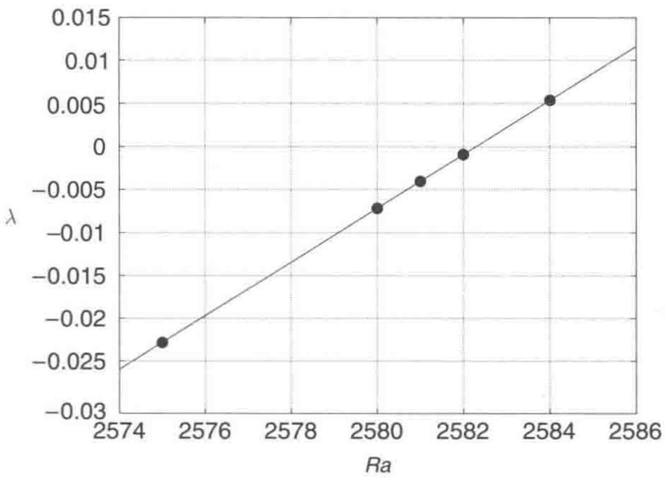


Figure 7 Temporal growth rate, λ, of infinitesimal perturbations, in the vicinity of the Hopf bifurcation of the quiescent state. Reproduced from Millour, Labrosse, and Tric (2003) *Physics of Fluids* 15(10): 2791–2802, with permission from American Institute of Physics.

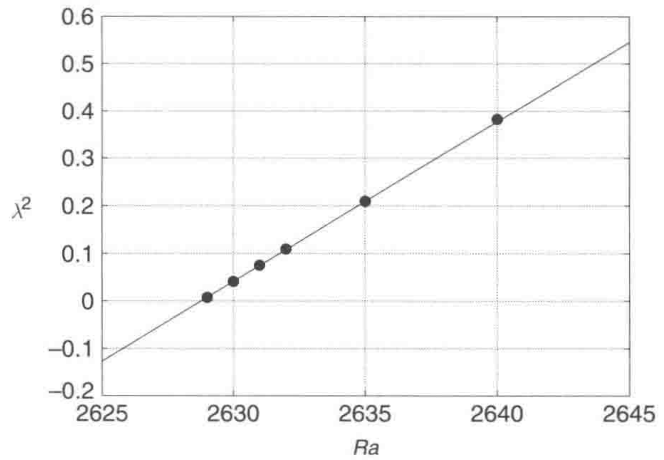


Figure 8 Squared temporal growth rate, λ^2, of transient relaxation towards the stationary state close to the saddle–node bifurcation. Reproduced from Millour, Labrosse, and Tric (2003) *Physics of Fluids* 15(10): 2791–2802, with permission from American Institute of Physics.

approximation of the flow in this midplane? Is it able to give a correct estimate of the two-dimensional flow stability within $\mathcal{D}$, and to predict the $\mathcal{D}$ frontiers, where the mirror-reflection symmetry property ceases to be valid? Only partial answers are available so far, coming from the thermally driven cubic cavity (**Figure 9**).

Filled with a pure fluid, its left and right vertical plates have fixed temperatures, T_0 ($\Theta = 0$ at $x = 0$) and $T_0 + \Delta T$ ($\Theta = 1$ at $x = 1$), while the others are adiabatic. Any $\Delta T \neq 0$ generates a flow, possibly mirror-symmetric about the vertical (hatched) midplane, and also centrosymmetric about $\hat{e}_y$. The two-dimensional approximation was extensively analyzed, numerically, with air as a fluid. A steady flow is obtained for $Ra < Ra_{2D,c} = (1.82 \pm 0.01) \times 10^8$,

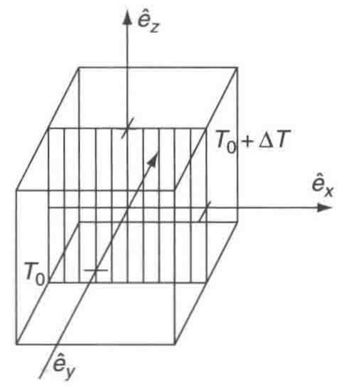


Figure 9 Sketch of the thermally driven cubic cavity.

where an oscillatory regime appears. The numerical three-dimensional flow is steady until $Ra_{3D,c} = 3.2 \times 10^7$, where it hysteretically bifurcates towards an oscillatory regime breaking the mirror symmetry about the midplane. Let us assess the validity of the two-dimensional approximate solutions. We define dimensionless heat fluxes (Nusselt numbers) which penetrate in one of the active walls,

$$Nu(y) = \int_0^1 \left.\frac{\partial \Theta_{3D}}{\partial x}\right|_{x=0} \mathrm{d}z$$

Three fluxes are interesting to compare: (1) in the midplane, $Nu_{\mathrm{mp}} = Nu(y = 1/2)$, (2) globally $Nu_{3D,W} = \int_0^1 Nu(y)\,\mathrm{d}y$, and (3) the two-dimensional approximation

$$Nu_{2D,W} = \int_0^1 \left.\frac{\partial \Theta_{2D}}{\partial x}\right|_{x=0} \mathrm{d}z$$

Figure 10 shows how they compare themselves, as a function of Ra. Quantitatively, the two-

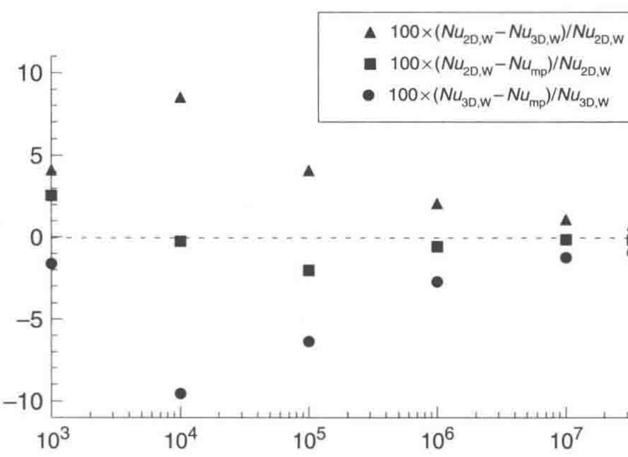


Figure 10 Relative 2D–3D Nusselt numbers. Reproduced with permission from Tric E, Labrosse G, and Betrouni M (2000) A first incursion into the 3D structure of natural convection of air in a differentially heated cubic cavity from accurate numerical solutions. *International Journal of Heat and Mass Transfer* 43: 4043–4056. © Elsevier Ltd.

dimensional approximation is not too bad, but not qualitatively, with a nonmonotonic evolution of the discrepancies. These latter become quite negligible when the three-dimensional flow gets unsteady and paradoxically loses the symmetry property on which its two-dimensional approximation is founded.

Thermocapillary Convection

Two immiscible liquids, or a liquid and a gas, are separated by a free surface, a region of small thickness (some ten molecular sizes). From a macroscopic viewpoint, it is considered as a singular entity. Its location and geometry are part of the solutions of the governing equations, themselves supposed to satisfy [20] on the free surface. As a first iteration, the free-surface shape can be imposed, fixed, and straight often.

Numerous industrial processes involve thermocapillarity wherein thermohydraulics involves complex phenomena, such as phase-change kinetics. A relevant modeling of these situations is a research subject by itself. For thermohydraulics, some academic configurations (**Figure 11**) have retained the attention of the scientific community.

Any thermohydraulic flow transfers heat between hot and cold solid boundaries wherein heat penetrates by conduction. Consequently, the term $(\vec{\nabla} \cdot \hat{t})\Theta$ of [20] never cancels at the solid boundary/free surface junction, as in **Figure 12**.

A nonzero vorticity is thus generated by thermocapillarity on the free surface until the wall, while flow adherence on the wall gives vorticity values of opposite sign. The problem presents therefore a vorticity singularity at the triple point. This is a deep physical and modeling problem.

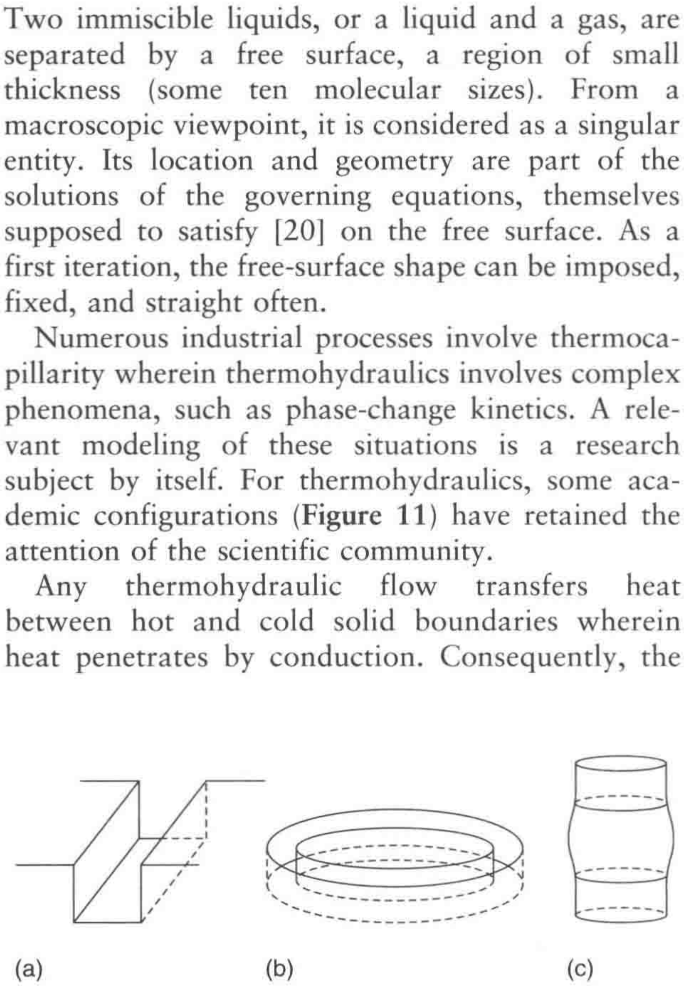


Figure 11 Open boat ((a) straight and (b) circular) and liquid bridge (c) configurations.

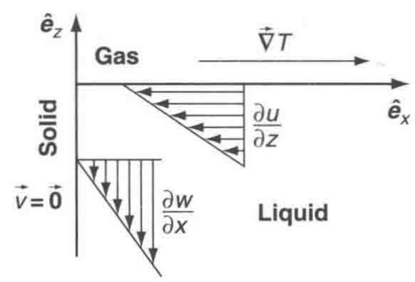


Figure 12 Thermocapillary origin of vorticity singularity (cold wall configuration).

See also: Bifurcations in Fluid Dynamics; Capillary Surfaces; Compressible Flows: Mathematical Theory; Dynamical Systems and Thermodynamics; Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; Fluid Mechanics: Numerical Methods; Magnetohydrodynamics; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Stability of Flows; Vortex Dynamics.

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Newtonian Limit of General Relativity

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Introduction

The general theory of relativity (GRT) unifies special relativity theory (SRT) and Newton's theory of gravitation (NGT). SRT and NGT describe successfully large domains of physical phenomena; therefore, one would like to understand how they survive as approximations in GRT.

In GRT, spacetime is idealized as a four-dimensional Lorentz manifold whose curvature is related to the distribution of energy and momentum. In such a spacetime, the existence of the exponential map implies that the metric near any event (spacetime point) x deviates from a flat metric only by terms given by the curvature there. Thus, if the gravitational tidal field, represented by the curvature tensor, is small near x, one may approximate the GR metric there by a flat Minkowski metric. This explains that SRT is a general local approximation to GRT. Apart from a remark at the end of the subsection "Local laws" the relation GRT $\rightarrow$ SRT will not be discussed further.

In its traditional formulation, Newton's theory differs drastically from Einstein's theory both in its spacetime structure and in its description of gravitation. The main purpose of this report is to show how NGT can nevertheless be understood as a kind of "limit" of GRT. More precisely, the structure of NGT can be viewed as a degenerate version of that of GRT, in parallel to the fact that the Galilei group can be obtained by contracting the Lorentz group.

In the next section we state the laws of GRT. We then reformulate these laws with slightly different field variables such that, besides the gravitational constant k, the speed of light appears via $\lambda = c^{-2}$. The resulting laws remain meaningful if λ and/or k are replaced by zero. They turn out to give a common basis for GRT, SRT, and NGT. The possibility of such a framework was indicated independently by Cartan (1923, 1924) and Friedrichs (1927) and extended by several authors; the complete formulation reviewed here was given by Ehlers (1981).

The section "Newton's theory in spacetime form" shows that the *laws* of NGT and SRT are obtained, with some additional restrictions, from the rescaled laws of GRT by putting, respectively, $\lambda = 0$ or $k = 0$. It is emphasized that Newton's theory proper is a theory only of isolated systems. Its intrinsic, four-dimensional formulation explains how the distinction between a vectorial gravitational field and inertial forces, as well as the existence of inertial frames, emerge as consequences of asymptotic flatness. These structures are lost in the so-called "Newtonian" cosmology whose dynamics is due to symmetry assumptions, whereas GR cosmology is a proper part of GRT.

The penultimate section is concerned with relations between *solutions* of GRT and NGT, and in the final section some results related to solutions are reported. They illustrate that the limit relation GRT $\rightarrow$ NGT may sometimes be inverted to get exact or approximate GR results from NGT. Approximations are related to uniform convergence in λ, as is indicated at the end of the final section.

The limit relations described here may be considered as a model for other theory relations in physics such as quantization or dequantization.

Notation Indices will be considered in general as "abstract" ones, characterizing the kind of objects independent of coordinate systems. Greek indices refer to spacetime, Latin ones to 3-space. Fields on spacetime will generally be taken to be smooth.

Basic Concepts and Laws of GRT

According to GRT, spacetime is a four-dimensional manifold M endowed with a Lorentzian metric $g_{\alpha\beta}$, here taken to have signature $(+ + + -)$. Any kind of matter including nongravitational fields is supposed to determine an energy tensor $T^{\alpha\beta}$. Metric and matter are interrelated by Einstein's gravitational field equation

$$R_{\alpha\beta} = \frac{8\pi k}{c^4}\left(T_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}T\right) \qquad [1]$$

In this equation, $T := T^{\alpha}{}_{\alpha}$ denotes the trace of the energy tensor, k and c stand for Newton's constant of gravity and the speed of light, respectively, and the Ricci tensor $R_{\alpha\beta}$ is obtained from Riemann's curvature tensor by contraction

$$R_{\alpha\beta} := R^{\gamma}{}_{\alpha\gamma\beta}$$

The curvature tensor is constructed from the symmetric, linear connection $\Gamma_{\beta}{}^{\alpha}{}_{\gamma}$ determined by the metric.

Equation [1] implies the vanishing of the covariant divergence of the energy tensor

$$T^{\alpha\beta}{}_{;\beta} = 0 \qquad [2]$$

the GRT analog of the laws of local conservation of energy and momentum.

The energy tensor depends on the kind of matter to be taken into account. In this article, only vacuum fields ($T^{\alpha\beta}=0$) and perfect fluids will be considered. For such a fluid,

$$T^{\alpha\beta} = (\rho + c^{-2}p)U^{\alpha}U^{\beta} + pg^{\alpha\beta} \qquad [3a]$$

ρ and p denote the mass density and the pressure, respectively, and the 4-velocity U^{α} is a timelike vector obeying

$$g_{\alpha\beta}U^{\alpha}U^{\beta} = -c^2 \qquad [3b]$$

If thermodynamical relations are added to specify the kind of fluid – the simplest cases are barotropic equations $p=f(\rho)$ – then eqns [1]–[3] admit a well-posed initial value problem for the fields $g_{\alpha\beta}, U^{\alpha}, \rho$.

Different matter models which could be treated in the context of this report are elastic bodies and ideal gases, but not point particles. Point particles fit into GRT even less than into electrodynamics.

The Cartan–Friedrichs Formalism

To obtain a spacetime formulation of NGT and a limit relation ART $\to$ NGT, we recall that the metric structure of Newton's spacetime consists of a scalar t, absolute time, which foliates M into instantaneous 3-spaces S_t, and Euclidean metrics $\gamma_{ab}(t)$ on these spaces. If the inverses $\gamma^{ab}(t)$ are pushed forward onto M via the embeddings $S_t \to M$, a field $s^{\alpha\beta}$ on M results which is assumed to be smooth. By construction,

$$s^{\alpha\beta}t_{,\beta} = 0 \qquad [4]$$

The pair $(t, s^{\alpha\beta})$ defines the "metric," that is, times and distances, in NGT.

Such a structure can arise from a Lorentzian metric, for example, the Minkowski metric $\eta_{\alpha\beta}$, by taking, component-wise, the limits

$$\begin{aligned} &-c^{-2}\eta_{\alpha\beta}\,dx^{\alpha}\,dx^{\beta} \\ &\quad\equiv dt^2 - c^{-2}\,dx^2 \underset{c\to\infty}{\longrightarrow} dt^2,\ \eta^{\alpha\beta} \underset{c\to\infty}{\longrightarrow} s^{\alpha\beta} \end{aligned} \qquad [5]$$

which can be interpreted geometrically as "opening up the light cones" until they degenerate into doubly covered, spacelike hyperplanes, the Newtonian S_t's.

The relations [5] suggest to write the GRT laws in terms of the rescaled temporal metric ($\lambda \equiv c^{-2}$)

$$t_{\alpha\beta} := -\lambda g_{\alpha\beta} \qquad [6]$$

and to write – presently only as a change of notation – $s^{\alpha\beta}$ instead of $g^{\alpha\beta}$. Then the fields $t_{\alpha\beta}, s^{\alpha\beta}, \Gamma_{\beta}{}^{\alpha}{}_{\gamma}, T^{\alpha\beta}, \rho, p, U^{\alpha}$, called the basic fields below, and constants $k>0, \lambda>0$ satisfy the following laws:

$$t_{\alpha\gamma}s^{\gamma\beta} = -\lambda\delta^{\beta}{}_{\alpha} \qquad [7a]$$

$$t_{\alpha\beta;\gamma} = 0, \qquad s^{\alpha\beta}{}_{;\gamma} = 0 \qquad [7b]$$

$$R^{\alpha}{}_{\beta}{}^{\gamma}{}_{\delta} = R^{\gamma}{}_{\delta}{}^{\alpha}{}_{\beta} \qquad [7c]$$

$$R_{\alpha\beta} = 8\pi k\left(t_{\alpha\gamma}t_{\beta\delta} - \frac{1}{2}t_{\alpha\beta}t_{\gamma\delta}\right)T^{\gamma\delta} \qquad [7d]$$

$$T^{\alpha\beta}{}_{;\beta} = 0 \qquad [7e]$$

$$T^{\alpha\beta} = (\rho + \lambda p)U^{\alpha}U^{\beta} + ps^{\alpha\beta} \qquad [7f]$$

$$t_{\alpha\beta}U^{\alpha}U^{\beta} = 1 \qquad [7g]$$

The Lorentz signature of $g_{\alpha\beta}$ can be reexpressed thus: at each event ($\cong$ spacetime point), there exists a "timelike" vector V^{α}, that is,

$$t_{\alpha\beta}V^{\alpha}V^{\beta} > 0 \qquad [7h]$$

and $V^{\alpha}X_{\alpha}=0$ for $X_{\alpha}\neq 0$ implies $s^{\alpha\beta}X_{\alpha}X_{\beta}>0$.

The indices in eqn [7c] are raised, here and later, by $s^{\alpha\beta}$.

Given a set of basic fields on M as listed below eqn [6], the laws [7] remain meaningful for all $\lambda \geq 0$ and $k \geq 0$. If $\lambda=0$, the "metrics" $t_{\alpha\beta}$ and $s^{\alpha\beta}$ degenerate (and the pair $(t_{\alpha\beta}, s^{\alpha\beta})$ is then called a Galilei metric). Nevertheless, the definition of "timelike" will also be used in that case. Also, X^{α} will be said to be "spacelike" if and only if it can be written $X^{\alpha}=s^{\alpha\beta}\xi_{\beta}$ with $s^{\alpha\beta}\xi_{\alpha}\xi_{\beta}>0$. While for $\lambda>0$, some of the relations [7] are redundant, this is not so for $\lambda=0$. For example, if $\lambda=0$, the two eqns [7b] are independent and do not determine the connection $\Gamma_{\beta}{}^{\alpha}{}_{\gamma}$ uniquely, in contrast to the case $\lambda>0$. The connection will always be assumed to be symmetric.

As will be discussed below, these formulas define a framework which serves to relate GRT to NGT and special relativity (SRT). First steps to formulate such a framework have been taken independently by E Cartan and KO Friedrichs. Therefore we call the structure defined by [7] the Cartan–Friedrichs formalism (CFF). We call it a "formalism" and not a "theory" since it is of interest solely as a tool to study relations between theories.

Equations [7] remain unchanged if the basic fields and constants are rescaled according to a change of units for time, length, and mass. Here, two sets of basic fields related by such a rescaling will be considered as physically equivalent; they provide the

same relations between observables. Thus, λ and k have no physical meanings, but only their signs:

$$\lambda > 0,\ k > 0: \quad \text{GRT}$$

$$\lambda = 0,\ k > 0: \quad \text{NGT}$$

$$\lambda > 0,\ k = 0: \quad \text{SRT}$$

(The last two lines are not sufficient to specify the theories within CFF; in connection with eqn [9] and in Theorem 2 they will be completed.) For discussing limit relations between theories, it is nevertheless useful to represent physical models in different scales.

The physical interpretation of $t_{\alpha\beta}, s^{\alpha\beta}$ in terms of time and distance and that of $\Gamma_\beta{}^\alpha{}_\gamma$ through its geodesics as world lines of freely falling test particles, respectively, is the same in the three theories and can be stated in terms of the common framework CFF.

For an obvious reason, λ may be called causality constant. Note that λ and k each occur in only one of the general laws of the theory, apart from the λ in [7f].

The laws [7] are invariant under diffeomorphisms of the spacetime manifold. Those diffeomorphisms which map the basic fields of a solution into themselves form the symmetry group of that solution.

Newton's Theory in Spacetime Form

Local Laws

Remarkably, for $\lambda = 0$ and $k > 0$ the formulas [7] reproduce *almost* all the laws on which Newton's theory of spacetime coupled to Euler's fluid theory is based. This is summarized in the following:

Theorem 1 *Let eqn* [7] *hold on M with $\lambda = 0$. Then there exists, for any event of M, a neighborhood U with coordinates (x^a, t) such that, on U, t coincides with the absolute time, $t_{\alpha\beta} = t_{,\alpha} t_{,\beta}$, and on the local slices $U \cap S_t$, $s^{\alpha\beta}$ defines Euclidean metrics γ_{ab} with orthonormal coordinates $x^a, \gamma_{ab} = \delta_{ab}$. Vectors are spacelike iff they are tangent to S_t, otherwise they are timelike. Moreover, the slices are locally geodesic with respect to the connection $\Gamma_\beta{}^\alpha{}_\gamma$, and the induced connection on the slices is the flat connection associated naturally to γ_{ab}. In addition, in the coordinate chart given by (x^a, t), the connection components vanish except $\Gamma_0{}^a{}_0$ and $\Gamma_0{}^b{}_a (= -\Gamma_0{}^a{}_b)$. Therefore, t is an affine parameter on timelike geodesics. Further, $U^0 = 1$, and $U^a = v^a$ is the 3-velocity of the fluid. If one writes*

$$-\Gamma_0{}^a{}_0 =: g^a, \qquad -\Gamma_0{}^a{}_b =: \omega^a{}_b \qquad [8a]$$

and uses 3-vector notation with $(g^a) = \boldsymbol{g}$, $(\omega_{23}, \omega_{31}, \omega_{12}) = \boldsymbol{\omega}$, the timelike geodesics of $\Gamma_\beta{}^\alpha{}_\gamma$ are given by

$$\ddot{\boldsymbol{x}} = \boldsymbol{g} + 2\dot{\boldsymbol{x}} \times \boldsymbol{\omega} \qquad [8b]$$

$\boldsymbol{g}$ and $\boldsymbol{\omega}$ satisfy

$$\nabla \cdot \boldsymbol{\omega} = 0, \quad \nabla \times \boldsymbol{g} + 2\dot{\boldsymbol{\omega}} = 0 \qquad [8c]$$

$$\nabla \times \boldsymbol{\omega} = 0,\ \nabla \cdot \boldsymbol{g} - 2\boldsymbol{\omega}^2 = -4\pi k \rho \qquad [8d]$$

and the fluid's equations of motion are

$$\dot{\rho} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \qquad [8e]$$

$$\rho(\dot{\boldsymbol{v}} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} - \boldsymbol{g} - 2\boldsymbol{v} \times \boldsymbol{\omega}) + \nabla p = 0 \qquad [8f]$$

A solution $(\boldsymbol{g}, \boldsymbol{\omega}, \rho, p, \boldsymbol{v})$ of eqns [8] *on a local chart (x^a, t) with $t_{\alpha\beta} = \text{diag}(0,0,0,1)$ and $s^{\alpha\beta} = \text{diag}(1,1,1,0)$ provides, via eqn* [8a], *the general local solution to eqns* [7] *for $\lambda = 0$.*

The proof consists of many, mostly elementary steps which can be gathered from Künzle (1972) and Ehlers (1981).

Given a solution to eqns (7) with $\lambda = 0$ and $k > 0$, the coordinates $x^\alpha = (x^a, t)$ referred to in the theorem are determined by the basic fields up to time-dependent Euclidean motions, time translations, and time reflections. Such a coordinate system corresponds to a rigid reference frame. As the equation of motion for freely falling particles, eqn [8b], shows, $\boldsymbol{g}$ and $\boldsymbol{\omega}$ are to be interpreted as the acceleration and rotation fields which determine, relative to a rigid frame, the combined influence of inertia and gravity on particles encoded in the spacetime connection $\Gamma_\beta{}^\alpha{}_\gamma$. (This role of a connection in NGT was recognized by E Cartan.) This interpretation is supported by the (generalized) Euler equation [8f].

As claimed above already, eqns [7] *almost* reproduce the local laws of the Newton–Euler theory. Indeed, eqns [8] are those of the Newton–Euler theory, provided $\boldsymbol{\omega}$ depends on time only. Then and only then can the coordinate freedom be used to get nonrotating rigid coordinates with respect to which $\boldsymbol{\omega} = 0$. The existence of such coordinates is indispensable for NGT since only with respect to them $-\boldsymbol{g}$ is the gradient of a potential U which obeys Poisson's equation, as shown by eqns [8c] and [8d].

The preceding argument shows that the CFF, specialized to $\lambda = 0$, has to be restricted by a condition which implies $\boldsymbol{\omega} = \boldsymbol{\omega}(t)$ in order to give the local laws of NGT. One such condition is

$$R^{\alpha\beta}{}_{\gamma\delta} = 0 \qquad [9]$$

as can be verified by computing the curvature tensor via eqn [8a].

Equation [9] for $\lambda=0$ expresses that parallel transport of spacelike vectors along arbitrary spacetime curves is integrable, which corresponds to the behavior of free gyroscopes in NGT (in contrast to GRT).

Of course, eqn [9] cannot be added to the CFF since it is incompatible with GRT. If, however, the CFF with $\lambda>0, k=0$ is restricted by the condition [9], the spacetime and hydrodynamics of special relativity result.

Global Laws for Isolated Systems

The laws [8] and [9] do not determine the time evolution of the basic fields. Using nonrotating coordinates we put $\boldsymbol{g}=-\nabla U$ and replace eqns [8c], [8d] by Poisson's equation

$$\Delta U=4\pi k\rho \qquad [10]$$

In Newtonian dynamics, the potential only serves to compute forces depending instantaneously on the mass distribution. Traditionally, this is achieved by assuming ρ to have spatially compact support at each time and to solve eqn [10] by

$$\phi(\boldsymbol{x},t)=-k\int\frac{\rho(\boldsymbol{x}+\boldsymbol{y},t)}{|\boldsymbol{y}|}\mathrm{d}^3y \qquad [11]$$

which implies the fall-off

$$\lim_{\substack{|\boldsymbol{x}|\to\infty,\\ t=\text{const.}}}\phi(\boldsymbol{x},t)=0 \qquad [12]$$

(ϕ will always be used for this solution of eqn [10]).

To relate the foregoing isolation assumptions to corresponding assumptions in GRT as far as presently possible, it seems necessary to go back to the laws [7] restricted to $\lambda=0$ or the equivalent $(3+1)$ version [8] without the restriction [9].

If some global assumptions are added to eqns [8], eqns [10]–[12] can be deduced from the four-dimensional formulation. One first introduces the following two assumptions:

(1) The hypersurfaces S_t of M (which, for $\lambda=0$, are the only spacelike hypersurfaces) are simply connected, complete Euclidean spaces.
(2) On each S_t, the support of ρ is compact.

Using coordinates (x^a,t) as in the last subsection, with x^a now ranging on $\mathbb{R}^3$, eqns [8a] imply

$$R^{\alpha}{}_{\beta\gamma\delta}R^{\beta}{}_{\alpha}{}^{\gamma}{}_{\epsilon}=-2\sum_{a,b}(\omega_{a,b})^2t_{\delta\epsilon} \qquad [13]$$

Hence the sum is a 4-scalar, and since $t_{\alpha\beta}$ is covariantly constant, it is possible to require

$$R^{\alpha}{}_{\beta\gamma\delta}R^{\beta}{}_{\alpha}{}^{\gamma}{}_{\epsilon}\to 0 \quad \text{at spatial infinity} \qquad [14]$$

which expresses covariantly that $\omega_{a,b}\to 0$. Since $\boldsymbol{\omega}$ is harmonic on S_t (by eqns [8c], [8d]), this in turn implies $\omega_{a,b}=0$; thus, $\boldsymbol{\omega}$ depends on t only; the asymptotic condition [14] and the local laws imply eqn [9].

We may therefore employ rigid, nonrotating coordinates, $\boldsymbol{\omega}=0$. Then, by eqns [8a], [8c], [8d] the connection coefficients take the form

$$\Gamma_{\beta}{}^{\alpha}{}_{\gamma}=t_{,\beta}t_{,\gamma}s^{\alpha\delta}U_{,\delta} \qquad [15]$$

and

$$R^{\lambda}{}_{\alpha\mu\beta}R^{\mu}{}_{\gamma\lambda\delta}=t_{,\alpha}t_{,\beta}t_{,\gamma}t_{,\delta}\sum_{a,b}\sum_{a,b}(U_{,ab})^2 \qquad [16]$$

As before, we require

$$R^{\lambda}{}_{\alpha\mu\beta}R^{\mu}{}_{\gamma\lambda\delta}\to 0 \qquad [17]$$

and conclude $U_{,ab}\to 0$. Since the Newtonian potential ϕ of ρ also has this fall-off and $U-\phi$ is harmonic on $S_t\cong\mathbb{R}^3$, the following conclusion can be obtained:

Lemma 1 *The laws* [8] *and the global conditions* (1)–(2), [14], [17] *imply: in rigid, nonrotating coordinates, the connection*

$$\Gamma_{\beta}{}^{\alpha}{}_{\gamma}-t_{,\beta}t_{,\gamma}s^{\alpha\delta}\phi_{,\delta}=\overset{\circ}{\Gamma}_{\beta}{}^{\alpha} \qquad [18]$$

is flat (ϕ according to eqn [11] *is a scalar, and the ϕ-term in eqn* [18] *is a tensor). In other words, $\Gamma_{\beta}{}^{\alpha}{}_{\gamma}$ is asymptotically flat since the ϕ-term falls of as $|\boldsymbol{x}|^{-2}$.*

Because of this lemma, one can further restrict the coordinates (x^a,t) by demanding $\overset{\circ}{\Gamma}_{\beta}{}^{\alpha}{}_{\gamma}=0$. In physical terms this means: by switching to a new, "unaccelerated" frame of reference, one removes from the equations of motion a spatially homogeneous gravitational field which, in contrast to the ϕ-term in eqn [16], is not due to matter.

The resulting coordinates are defined, up to Galilean transformations,

$$t'=\pm t+c^{0'}$$
$$x^{a'}=D^{a'}{}_{b}x^b+u^{a'}t+c^{a'}$$

where $c^{a'}, u^{a'}$ are constants and D is a constant orthogonal 3×3 matrix. These coordinates are called inertial ones; with respect to them the usual laws of Newtonian mechanics hold; see [8] with $\boldsymbol{\omega}=0$ and $U=\phi[\rho]$.

Theorem 2 (Ehlers 1981). *The laws* [7] *of the CFF restricted to $\lambda=0$ and augmented by the global and asymptotic conditions* (1)–(2), [14], [17], *provide a generally covariant, four-dimensional*

formulation for the Newtonian theory of space, time, gravitation, and hydrodynamics.

The possibility to split the connection Γ into a flat part which is independent of matter and a tensorial part depending on matter and given by the vector field $g^\alpha = s^{\alpha\beta}\phi_{,\beta}$ (with ϕ from eqn [11]), arises only from supplementing the local laws [7] by the global, resp. asymptotic, conditions (1)–(2), [14], [17] stated above. The introduction of inertial coordinates is then convenient, but not necessary. In noninertial, rigid frames of reference, $\overset{\circ}{\Gamma}{}_\beta{}^\alpha{}_\gamma$ gives rise to inertial forces.

It should be possible to define spatial asymptotic flatness in the CFF, but that has not been done.

Remarks on Newtonian Cosmology

In cosmology, the conditions (2) and [17] of the last subsection are not appropriate. Instead one keeps the laws [7] and adds to them eqn [9], so that with respect to nonrotating coordinates the laws [8] with $\boldsymbol{\omega} = 0$ and eqn [10] remain valid. Then, there are no longer inertial coordinate systems, and the potential U is not a 4-scalar. For a slightly different approach, see Rüede and Straumann (1997).

For the purpose of this article, the term "cosmological model" will be applied to those solutions of the laws [7] and [9] which satisfy $\rho > 0$ and which have a symmetry group which acts transitively on the set of world lines representing the motion of the fluid. This strong symmetry assumption determines the time-evolution even in the "Newtonian" case $\lambda = 0$ in spite of the absence of an evolution equation for the gravitational field g.

Newtonian Limits of Families of GR Solutions

The discussion in the sections "The Cartan–Friedrichs formalism" and "Newton's theory in spacetime form" suggests the following:

Definition 1 Let a family $\mathcal{F}(\lambda) = (t_{\alpha\beta}(\lambda), \ldots)$ of basic fields parametrized by λ, obeying the laws [7] of the CFF, be given for $0 \le \lambda < a$. We assume the underlying manifolds $M(\lambda)$ to be open submanifolds of a fixed manifold M such that $M(\lambda_1) \supseteq M(\lambda_2)$ if $\lambda_1 < \lambda_2$ and $\bigcup_\lambda M(\lambda) = M$. Then we write

$$\lim_{\lambda \to 0} \mathcal{F}(\lambda) = \mathcal{F}(0) \qquad [19]$$

if the fields of $\mathcal{F}(\lambda)$ and their first derivatives converge pointwise to those of $\mathcal{F}(0)$.

$\mathcal{F}(0)$ is then said to be a CF limit of the sequence of (λ-rescaled) solutions $\mathcal{F}(\lambda)$ of GRT. If the fields of a λ-family of GR solutions ($\lambda > 0$) and their first derivatives converge for $\lambda \to 0$ locally uniformly, then the limit fields satisfy eqns [7]. If $\mathcal{F}(0)$ has the additional property [9], the limit is locally Newtonian.

On the basis of the section "The Cartan–Friedrichs formalism" one may conjecture that if eqn [19] holds and the $\mathcal{F}(\lambda)$ for $\lambda > 0$ are spatially asymptotically flat, $\mathcal{F}(0)$ will represent an asymptotically flat Newtonian spacetime. Examples such as Example 1 below are in agreement with this conjecture, but a general proof is not known.

Example 1 The interior solution for a static, spherically symmetric fluid ball of constant energy density (Schwarzschild 1916) is given by

$$ds^2 = \frac{dr^2}{a^2} + r^2(d\vartheta^2 + \sin^2\vartheta \, d\varphi^2) - \frac{1}{4}(3a_0 - a)^2 c^2 \, dt^2$$

$$\rho = \text{const.} > 0, \qquad p = \rho c^2 \frac{a - a_0}{3a_0 - a}$$

$$U = \frac{2}{3a_0 - a}\partial_t, \quad a(r) = \left(1 - \frac{8\pi}{3} k c^{-2} r^2 \rho\right)^{1/2}$$

$$a_0 = a(r_0)$$

Inserting into these expressions the parameter $\lambda = c^{-2}$ and treating ρ and r_0 as λ-independent constants results in a λ-family with $0 \le \lambda < ((8\pi/3)kr_0^3\rho)^{-1}$. The limit solution represents a Newtonian fluid ball of constant mass density ρ. The Schwarzschild vacuum fields belonging to these fluid balls also have the appropriate Newtonian limits. The resulting complete spacetimes are asymptotically flat. A dimensionless small parameter which could be used instead of λ to measure the deviation of the GR solution from its Newtonian limit is the ratio of Schwarzschild radius and the geometric radius:

$$\frac{2kM}{c^2 r_0} = \frac{8\pi}{3}\frac{k\rho r_0^2}{c^2}$$

Example 2 A Friedmann–Lemaitre cosmological model of GR containing dust and radiation is given by

$$ds^2 = R^2(t)\frac{\delta_{ab} d\xi^a d\xi^b}{(1 - (1/4)(E/c^2)\delta_{ab}\xi^a\xi^b)^2} - c^2 dt^2$$

where $R(t)$ obeys

$$\dot{R}^2 - \frac{8\pi}{3}k\left(\frac{M}{R} + \frac{S}{c^2 R^2}\right) = E$$

M is a mass constant, $\rho = M/R^3$ is the mass density of "dust," S is an entropy constant, $\epsilon = S/R^4$ the energy density and $p = (1/3)\epsilon$ the pressure of radiation; and E is a constant of dimension $(\text{speed})^2$. The world lines of the fluid elements are given by $\xi^a = \text{const.}$ (Lagrangian comoving coordinates).

Taking E, M, S constant and $\lambda = c^{-2}$ as a parameter provides a λ-family of GR models with Newtonian limit. In the limit, t is the Newtonian time, and the spatial metric $R^2\delta_{ab}\mathrm{d}\xi^a\mathrm{d}\xi^b$ describes an expanding Euclidian space $\mathbb{R}^3$ (if $E \leq 0$) or an open ball of radius $2R(t)$ in it (if $E > 0$). In the coordinates (ξ^a, t) the connection does not have the "Newtonian" components [8a], instead its nonvanishing components are $\Gamma_0{}^a{}_b = (\dot{R}/R)\delta^a_b$. In local inertial coordinates $x^a = R\xi^a$ centered on the particle with $\xi^a = 0$ (which could be any particle because of the homogeneity of the model), the spatial metric is $\mathrm{d}\boldsymbol{x}^2$, and the connection components are Newtonian, with $U = (2\pi/3)k\rho\boldsymbol{x}^2$ and $\Delta U = 4\pi k\rho$. In the limit, the radiation no longer influences the expansion; one gets the Newtonian dust models (eqn [9] is satisfied). The connection is, of course, not asymptotically flat. The curvature tensor $R^\alpha{}_\beta{}^\gamma{}_\delta = (4\pi/3)k\rho t_{\beta\delta}s^{\alpha\gamma}$ exhibits homogeneity and isotropy. The Gaussian sectional curvature of the 3-space at time t is $K = -\lambda E/R^2$. As a dimensionless smallness parameter one can take E/c^2. In the "open" models, with $E \geq 0$, the coordinates ξ^a cover the whole 3-manifold of fluid particles, while in the "closed" case, $E < 0$, one particle, the antipode of $\xi^a = 0$ on the 3-sphere, is not covered. That particle is missing in the Newtonian limit model. In the Newtonian case the expanding Euclidian space $\mathbb{R}^3$ can be replaced by a torus; in the GR cases this is possible only for $E = 0$.

Many examples of GR families with Newtonian limits are known (see, e.g., Ehlers (1997) and references therein). An example of a λ-family which has an almost Newtonian limit which does not satisfy eqn [9] is provided by NUT spacetimes (see Ehlers 1997), interpreted as due to a gravitomagnetic monopole (Lynden-Bell and Nouri-Zonez 1998).

Applications and Problems

Can one construct, for a given Newtonian solution N, a λ-family of GR solutions which converges to N? Some answers are known and listed below.

U Heilig (1995) has shown: given a solution to the Euler–Poisson equations representing a stationary, rigidly rotating, self-gravitating fluid body with its surrounding gravitational field, there exists a λ-family of corresponding solutions to the Einstein–Euler system having the given solutions as its limit.

The proof is based on the fact that one can reformulate eqns [1], [2] in terms of harmonic coordinates and new dependent gravitational variables instead of $g_{\alpha\beta}$ such that the new equations given in Lottermoser (1992) are analytic in λ and reduce, for $\lambda = 0$, to the Euler–Poisson system. In the stationary case these equations are elliptic for $\lambda \geq 0$. Using appropriate function spaces, Heilig shows, via the implicit function theorem, that a solution for $\lambda = 0$ can be extended to small, positive values of λ. Since L Lichtenstein has constructed solutions as assumed in the theorem, the existence of GR solutions follows.

The gravitational part of the system of equations referred to above is hyperbolic for $\lambda > 0$, but becomes elliptic for $\lambda = 0$, whereas the fluid equations remain hyperbolic. In spite of this difficulty Rendall (1994) has shown that λ-families of time-dependent, asymptotically flat solutions to the Einstein–Vlasov system representing gravitating systems of collisionless particles have Poisson–Vlasov limits, and that any Poisson–Vlasov solution can be so obtained.

Lottermoser (1992) succeeded in proving the existence of λ-families of solutions to the Einstein constraint equations which have Newtonian initial data as limits. Nothing seems to be known about solutions evolving from such data. Lottermoser has given an interesting discussion concerning possible extension of his work which apparently has gone unnoticed.

Rendall (1992) has defined and analyzed post-Newtonian expansions to Einstein's equations and their solvability, assuming λ-families whose $t_{\alpha\beta}, s^{\alpha\beta}$ are a few times differentiable in $\epsilon = \sqrt{\lambda}$ at $\epsilon = 0$. He found that for low orders the equations have asymptotically flat solutions, but that at order ϵ^8 divergences occur for general Newtonian seed solutions. Modifications of the method to overcome these difficulties have been considered by Rendall and others; the problem is open.

In cosmology, one uses homogeneous background models and studies their perturbations. The latter are frequently based on Newtonian equations. This can perhaps be justified as follows. According to Example 2 the fields of Friedmann–Lemaitre models differ from their Newtonian limits by arbitrarily small amounts uniformly in spacetime regions where the terms involving λ are small, that is,

$$\frac{S}{Mc^2} \ll R(t), \quad \frac{\sqrt{|E|}}{c}|\boldsymbol{x}| \ll R(t)$$

Additional conditions will be needed to ensure that Newtonian perturbations approximate relativistic ones and that gravitational wave perturbations can be neglected.

See also: Cosmology: Mathematical Aspects; Einstein Equations: Exact Solutions; General Relativity: Overview; Gravitational Lensing; Shock Wave Refinement of the Friedman–Robertson–Walker Metric.

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Noncommutative Geometry and the Standard Model

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Introduction

The aim of this contribution is to explain how Connes derives the standard model of electromagnetic, weak, and strong forces from noncommutative geometry. The reader is supposed to be aware of two other derivations in fundamental physics: the derivation of the Balmer–Rydberg formula for the spectrum of the hydrogen atom from quantum mechanics and Einstein's derivation of gravity from Riemannian geometry.

At the end of the nineteenth century, new physics was discovered in atoms, namely their discrete spectra. Balmer and Rydberg succeeded to put order into the fast-growing set of experimental results with the help of a phenomenological ansatz for the frequencies ν of the spectral rays of, for example, the hydrogen atom,

$$\nu = g(n_2^q - n_1^q), \quad n_j \in \mathbb{N}, \ q \in \mathbb{Z}, \ g \in \mathbb{R} \qquad [1]$$

The integer variables n_1 and n_2 reflect the discreteness of the spectrum. On the other hand, the discrete parameter q and the continuous parameter g were fitted by experiment: $q = -2$ and $g = 3.289 \times 10^{15}$ Hz, the famous Rydberg constant. Later quantum mechanics was discovered and allowed to derive the Balmer–Rydberg ansatz and to constrain its parameters:

$$q = 2 \quad \text{and} \quad g = \frac{m_e}{4\pi\hbar^3}\frac{e^4}{(4\pi\epsilon_0)^2} \qquad [2]$$

in beautiful agreement with the anterior experimental fit.

The Standard Model

We propose to introduce the standard model (*see* Standard Model of Particle Physics) in analogy with the Balmer–Rydberg formula (**Table 1**).

Table 1 An analogy between atomic and particle physics elements

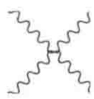
	Atomic physics	*Particle physics*
New physics	Discrete spectra	Forces mediated by gauge bosons
Ansatz	$\nu = g(n_2^q - n_1^q)$	Yang–Mills–Higgs models
Experimental fit	$q = -2, g = 3.289 \times 10^{15}$ Hz	Standard model
Underlying theory	Quantum mechanics	Noncommutative geometry

The Yang–Mills–Higgs Ansatz

The variables of this Lagrangian ansatz are spin-1 particles A, spin-(1/2) particles decomposed into left- and right-handed components $\psi = (\psi_L, \psi_R)$ and spin-0 particles φ. There are four discrete parameters, a compact real Lie group G, the "gauge group," and three unitary representations on complex Hilbert spaces $\mathcal{H}_L, \mathcal{H}_R$, and $\mathcal{H}_S$. The spin-1 particles come in a multiplet living in the complexified of the Lie algebra of G, $A \in \mathrm{Lie}(G)^{\mathbb{C}}$. The left- and right-handed spinors come in multiplets living in the Hilbert spaces, $\psi_L \in \mathcal{H}_L, \psi_R \in \mathcal{H}_R$, respectively. The (Higgs) scalar is another multiplet, $\varphi \in \mathcal{H}_S$. The Yang–Mills–Higgs Lagrangian, together with its Feynman diagrams, is spelled out in **Table 2**.

There are several continuous parameters: the gauge coupling $g \in \mathbb{R}_+$, the Higgs self-couplings $\lambda, \mu \in \mathbb{R}_+$, and several Yukawa couplings $g_Y \in \mathbb{C}$.

Table 2 The Yang–Mills–Higgs Lagrangian and its Feynman diagrams

Term	Diagram
$\mathcal{L}[A, \psi, \varphi] = \frac{1}{2}\mathrm{tr}(\partial_\mu A_\nu \partial^\mu A^\nu - \partial_\mu A_\nu \partial^\nu A^\mu)$	
$+g\ \mathrm{tr}(\partial_\mu A_\nu [A^\mu, A^\nu])$	
$+g^2\ \mathrm{tr}([A_\mu, A_\nu][A^\mu, A^\nu])$	
$+\bar{\psi}\partial\!\!\!/\psi$	
$+ig\bar{\psi}(\tilde{\rho}_L \oplus \tilde{\rho}_R)(A_\mu)\gamma^\mu\psi$	
$+\frac{1}{2}\partial_\mu\varphi^*\partial^\mu\varphi$	
$+\frac{1}{2}g\{(\tilde{\rho}_S(A_\mu)\varphi)^*\partial^\mu\varphi + \partial_\mu\varphi^*\tilde{\rho}_S(A_\mu)\varphi\}$	
$+\frac{1}{2}g^2(\tilde{\rho}_S(A_\mu)\varphi)^*\tilde{\rho}_S(A^\mu)\varphi$	
$+\lambda\varphi^*\varphi\varphi^*\varphi$	
$-\frac{1}{2}\mu^2\varphi^*\varphi$	
$+g_Y\ \bar{\psi}\varphi\psi + \bar{g}_Y\ \bar{\psi}\varphi^*\psi$	

Let us choose $G = U(1) \ni e^{i\theta}$. Its irreducible unitary representations are all one-dimensional, $\mathcal{H} = \mathbb{C} \ni \psi$ characterized by the charge $q \in \mathbb{Z}$: $\rho(e^{i\theta})\psi = e^{iq\theta}\psi$. Then with $q_L = q_R$ and $\mathcal{H}_S = \{0\}$, we get Maxwell's theory with the photon (or gauge boson or 4-potential) A coupled to the Dirac theory of a massless spinor of electric charge q_L whose (relativistic) wave function is ψ. The gauge coupling is given by $g = e/\sqrt{\epsilon_0}$. Gauge invariance of the Yang–Mills–Higgs Lagrangian implies, via Noether's theorem, electric charge conservation in this case (*see* Symmetries and Conservation Laws).

Yang–Mills models are therefore simply nonabelian generalizations of electromagnetism where the abelian gauge group U(1) is replaced by any compact real Lie group. We insist on a compact group because all irreducible unitary representations of compact groups are finite dimensional. Finally, the Higgs scalar is added to give masses to spinors and gauge bosons via spontaneous symmetry breaking (*see* Symmetry Breaking in Field Theory).

We use compact groups and unitary representations as (discrete) parameters. One motivation is Noether's theorem and conserved quantities. The other comes from Wigner's theorem: the irreducible unitary representations of the Poincaré group are classified by mass and spin. Its orthonormal basis vectors are classified by energy–momentum and by the z-component of angular momentum. This theorem leads to the widely accepted definition of a particle as an orthonormal basis vector in a Hilbert space $\mathcal{H}$ carrying a unitary representation ρ of a group G.

A precious property of the Yang–Mills–Higgs ansatz is its perturbative renormalizability necessary for fine-structure calculations like the anomalous magnetic moment of the muon.

The Experimental Fit

Physicists have spent some 30 years and some 10^9 Swiss Francs to distill the fit (Particle Data Group 2004):

$$G = SU(2) \times U(1) \times SU(3)/(\mathbb{Z}_2 \times \mathbb{Z}_3) \quad [3]$$

$$\mathcal{H}_L = \bigoplus_1^3 [(2, \tfrac{1}{6}, 3) \oplus (2, -\tfrac{1}{2}, 1)] \quad [4]$$

$$\mathcal{H}_R = \bigoplus_1^3 [(1, \tfrac{2}{3}, 3) \oplus (1, -\tfrac{1}{3}, 3) \oplus (1, -1, 1)] \quad [5]$$

$$\mathcal{H}_S = (2, -\tfrac{1}{2}, 1) \quad [6]$$

Here (n_2, y, n_3) denotes the tensor product of an n_2-dimensional representation of SU(2), "(weak) isospin," an n_3-dimensional representation of SU(3), "color," and the one-dimensional representation of

U(1) with "hyper charge" y. For historical reasons, the hypercharge is an integer multiple of 1/6. This is irrelevant: in the abelian case, only the product of the hypercharge with its gauge coupling is measurable, and we do not need multivalued representations, which are characterized by noninteger, rational hypercharges. In the direct sum, we recognize the three generations of fermions, the quarks, "up, down, charm, strange, top, bottom," are SU(3) triplets, the leptons, "electron, μ, τ" and their neutrinos, are color singlets. The basis of the fermion representation space is

$$\begin{pmatrix} u \\ d \end{pmatrix}_L, \quad \begin{pmatrix} c \\ s \end{pmatrix}_L, \quad \begin{pmatrix} t \\ b \end{pmatrix}_L$$
$$\begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \quad \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L$$
$$u_R, c_R, t_R, e_R, \mu_R, \tau_R$$
$$d_R, s_R, b_R,$$

The parentheses indicate isospin doublets.

The eight gauge bosons associated with su(3) are called gluons. Warning: the U(1) is not the one of electric charge; it is called hypercharge, the electric charge is a linear combination of hypercharge and weak isospin. This mixing is necessary to give electric charges to the W bosons. The W^+ and W^- are pure isospin states, while the Z^0 and the photon are (orthogonal) mixtures of the third isospin generator and hypercharge.

As the group G contains three simple factors, there are three gauge couplings,

$$g_2 = 0.6518 \pm 0.0003$$
$$g_1 = 0.3574 \pm 0.0001 \qquad [7]$$
$$g_3 = 1.218 \pm 0.01$$

The Higgs couplings are usually expressed in terms of the W and Higgs masses:

$$m_W = \tfrac{1}{2} g_2 v = 80.419 \pm 0.056\,\text{GeV} \qquad [8]$$

$$m_\varphi = 2\sqrt{2}\sqrt{\lambda} v > 98\,\text{GeV} \qquad [9]$$

with the vacuum expectation value $v := (1/2)\mu/\sqrt{\lambda}$. Because of the high degree of reducibility of the spin-(1/2) representations there are 27 complex Yukawa couplings. They constitute the fermionic mass matrix which contains the fermion masses and mixings:

$$m_e = 0.510998902 \pm 0.000000021\,\text{MeV}$$
$$m_u = 3 \pm 2\,\text{MeV}, \quad m_d = 6 \pm 3\,\text{MeV}$$
$$m_\mu = 0.105658357 \pm 0.000000005\,\text{GeV}$$
$$m_c = 1.25 \pm 0.1\,\text{GeV}, \quad m_s = 0.125 \pm 0.05\,\text{GeV}$$
$$m_\tau = 1.77703 \pm 0.00003\,\text{GeV}$$
$$m_t = 174.3 \pm 5.1\,\text{GeV}, \quad m_b = 4.2 \pm 0.2\,\text{GeV}$$

For simplicity, we have taken massless neutrinos. Then mixing only occurs for quarks and is given by a unitary matrix, the Cabibbo–Kobayashi–Maskawa matrix

$$C_{KM} := \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \qquad [10]$$

whose matrix elements in terms of absolute values are:

$$\begin{pmatrix} 0.9750 \pm 0.0008 & 0.223 \pm 0.004 & 0.004 \pm 0.002 \\ 0.222 \pm 0.003 & 0.9742 \pm 0.0008 & 0.040 \pm 0.003 \\ 0.009 \pm 0.005 & 0.039 \pm 0.004 & 0.9992 \pm 0.0003 \end{pmatrix} \qquad [11]$$

Mathematically, the Cabibbo–Kobayashi–Maskawa matrix comes from a polar decomposition of the mass matrix. The physical meaning of the quark mixings is the following: when a sufficiently energetic W^+ decays into a u quark, this u quark is produced together with a $\bar{d}$ quark with probability $|V_{ud}|^2$, an $\bar{s}$ quark with probability $|V_{us}|^2$, and a $\bar{b}$ quark with probability $|V_{ub}|^2$.

The phenomenological success of the standard model is phenomenal: with only a handful of parameters, it reproduces correctly some millions of experimental numbers: cross sections, lifetimes, branching ratios.

Noncommutative Geometry

Noncommutative geometry is an analytic geometry generalizing three other geometries that also had important impact on our understanding of forces and time. Let us start by briefly recalling the three forerunners (**Table 3**). Euclidean geometry underlies Newton's mechanics as a geometry in the space of positions. Forces are described by vectors living in the same space and the Euclidean scalar product is needed to define work and potential energy. Time is not part of geometry – it is absolute. This point of view is abandoned in special relativity unifying space and time into Minkowskian geometry. This new point of view allows to derive the magnetic

Table 3 Four nested analytic geometries

Geometry	*Force*	*Time*
Euclidean	$E = \int \vec{F} \cdot d\vec{x}$	Absolute
Minkowskian	$\vec{E}, \epsilon_0 \Rightarrow \vec{B}, \mu_0 = \epsilon_0^{-1} c^{-2}$	Universal
Riemannian	Coriolis $\leftrightarrow$ gravity	Proper, τ
Noncommutative	Gravity $\Rightarrow$ YMH, $\lambda = \frac{1}{3} g_2^2$	$\Delta\tau \sim 10^{-40}$ s

field from the electric field as a pseudoforce associated with a Lorentz boost. Although time becomes relative, one can still imagine a grid of synchronized clocks, that is, a universal time. The next generalization is "Riemannian geometry = curved spacetime." Here gravity can be viewed as the pseudoforce associated with a uniformly accelerated coordinate transformation. At the same time, universal time loses all meaning and we must content ourselves with proper time. With today's precision in time measurement, this complication of life becomes a bare necessity, for example, the global positioning system (GPS).

Our last generalization is "noncommutative geometry = curved space(time) with an uncertainty principle." As in quantum mechanics, this uncertainty principle is introduced via noncommutativity.

Quantum Mechanics

Consider the classical harmonic oscillator. Its phase space is $\mathbb{R}^2$ with points labeled by position x and momentum p. A classical observable is a differentiable function on phase space such as the total energy $p^2/(2m) + kx^2$. Observables can be added and multiplied, and they form the algebra $\mathcal{C}^\infty(\mathbb{R}^2)$, which is associative and commutative. To pass to quantum mechanics, this algebra is rendered noncommutative by means of a noncommutation relation for the generators x and p: $[x,p] = i\hbar 1$. Let us call $\mathcal{A}$ the resulting algebra "of quantum observables." It is still associative, and has an involution $\cdot^*$ (the adjoint or Hermitian conjugation) and a unit 1.

Of course, there is no space anymore of which $\mathcal{A}$ is the algebra of functions. Nevertheless, we talk about such a "quantum phase space" as a space that has no points or a space with an uncertainty relation. Indeed, the noncommutation relation implies Heisenberg's uncertainty relation $\Delta x \Delta p \geq \hbar/2$ and tells us that points in phase space lose all meaning; we can only resolve cells in phase space of volume $\hbar/2$, see **Figure 1**. To define the uncertainty Δa for an observable $a \in \mathcal{A}$, we need a faithful representation of the algebra on a Hilbert space, that is, an injective homomorphism ρ from $\mathcal{A}$ into the algebra of operators on $\mathcal{H}$. For the harmonic oscillator, this Hilbert space is $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$. Its elements are the wave functions $\psi(x)$, square-integrable functions on configuration space. Finally, the dynamics is defined by the Hamiltonian, a self-adjoint observable $H = H^* \in \mathcal{A}$ via Schrödinger's equation $(i\hbar\partial/\partial t - \rho(H))\psi(t,x) = 0$. Here time is an external parameter; in particular, time is not an observable. This is different in the special-relativistic setting, where Schrödinger's equation is replaced by Dirac's equation $\partial\!\!\!/\psi = 0$. Now the wave function ψ is the four-component spinor consisting of left- and right-handed, particle and antiparticle wave functions. Unlike the Hamiltonian, the Dirac operator does not lie in $\mathcal{A}$, but it is still an operator on $\mathcal{H}$. In Euclidean spacetime, the Dirac operator is also self-adjoint, $\partial\!\!\!/^* = \partial\!\!\!/$.

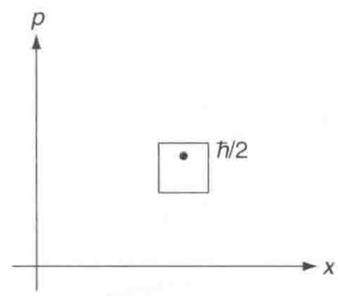


Figure 1 The first example of noncommutative geometry.

Spectral Triples

Noncommutative geometry (Connes 1994, 1995) does to a compact Riemannian spin manifold M what quantum mechanics does to phase space. A noncommutative geometry is defined by the three purely algebraic items $(\mathcal{A}, \mathcal{H}, \partial\!\!\!/)$, called a spectral triple. $\mathcal{A}$ is a real, associative, and possibly noncommutative involution algebra with unit, faithfully represented on a complex Hilbert space $\mathcal{H}$, and $\partial\!\!\!/$ is a self-adjoint operator on $\mathcal{H}$. As the spectral triple, also the axioms linking its three items are motivated by relativistic quantum mechanics.

When $\mathcal{A} = \mathcal{C}^\infty(M)$, the functions on a Riemannian spin manifold M, represented on spinors ψ, and $\partial\!\!\!/$ is the gravitational Dirac operator, one has a spectral triple. The converse is also true when $\mathcal{A}$ is a suitable commutative algebra (Connes 1996), but the axioms make sense even when $\mathcal{A}$ is not commutative. As for quantum phase space, Connes defines a noncommutative geometry by a spectral triple whose algebra is allowed to be noncommutative and he shows how important properties like dimensions, distances, differentiation, integration, general coordinate transformations, and direct products generalize to the noncommutative setting. As a bonus, the algebraic axioms of a spectral triple, commutative or not, include discrete, that is, zero-dimensional spaces that now are naturally equipped with a differential calculus. These spaces have finite-dimensional algebras and Hilbert spaces, meaning that their algebras are just matrix algebras.

An "almost commutative geometry" is defined as a direct product of a four-dimensional commutative geometry, "ordinary spacetime," by a zero-dimensional noncommutative geometry, the "internal space." If the

latter is also commutative, for example, the ordinary two-point space, then the direct product describes a two-sheeted universe or a Kaluza–Klein space whose fifth dimension is discrete, (Madone 1995). In general, the axioms of spectral triples imply that the Dirac operator of the internal space is precisely the fermionic mass matrix.

As a generic example, here is the internal spectral triple underlying the standard model with one generation of quarks and leptons. The algebra $\mathcal{A} = \mathbb{H} \oplus \mathbb{C} \oplus M_3(\mathbb{C}) \ni (a, b, c)$ contains quaternions, that is, 2×2 matrices of the form

$$a = \begin{pmatrix} x & -\bar{y} \\ y & \bar{x} \end{pmatrix}, \quad x, y \in \mathbb{C}$$

complex numbers b and complex 3×3 matrices c. The Hilbert space is 30-dimensional, where we count particles and antiparticles $(\cdot^c)$ separately: $\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_R \oplus \mathcal{H}_L^c \oplus \mathcal{H}_R^c = \mathbb{C}^8 \oplus \mathbb{C}^7 \oplus \mathbb{C}^8 \oplus \mathbb{C}^7$. The representation is block-diagonal, with the four blocks

$$\rho_L(a) := \begin{pmatrix} a \otimes 1_3 & 0 \\ 0 & a \end{pmatrix}$$
$$\rho_R(b) := \begin{pmatrix} b1_3 & 0 & 0 \\ 0 & \bar{b}1_3 & 0 \\ 0 & 0 & \bar{b} \end{pmatrix} \qquad [12]$$

$$\rho_L^c(b, c) := \begin{pmatrix} 1_2 \otimes c & 0 \\ 0 & \bar{b}1_2 \end{pmatrix}$$
$$\rho_R^c(b, c) := \begin{pmatrix} c & 0 & 0 \\ 0 & c & 0 \\ 0 & 0 & \bar{b} \end{pmatrix} \qquad [13]$$

The internal Dirac operator (= fermionic mass matrix) contains two quark masses m_u, m_d and one lepton mass m_e, and no mixing:

$$\mathcal{D} = \begin{pmatrix} 0 & \mathcal{M} & 0 & 0 \\ \mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{\mathcal{M}} \\ 0 & 0 & \bar{\mathcal{M}}^* & 0 \end{pmatrix}$$
$$\mathcal{M} = \begin{pmatrix} \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix} \otimes 1_3 & 0 \\ 0 & \begin{pmatrix} 0 \\ m_e \end{pmatrix} \end{pmatrix} \qquad [14]$$

These matrices look rather *ad hoc*; they are not. They define an irreducible spectral triple and, for a given algebra, there is only a finite number of such triples.

The Spectral Action

Chamseddine and Connes (1997) generalize general relativity to noncommutative spacetimes in two strokes, kinematics and dynamics. They explicitly compute this generalization for almost commutative geometries.

Kinematics In noncommutative geometry, general coordinate transformations are algebra automorphisms lifted to the Hilbert space of spinors. For almost commutative geometries, these transformations are precisely general coordinate transformations of ordinary spacetime and gauge transformations. Now remember how Einstein uses the equivalence principle to produce "gravity = curvature" starting from the flat metric, which in Connes' language is the ordinary flat Dirac operator. When applied to an almost commutative geometry (Connes 1996), the equivalence principle produces again a curved metric via the ordinary coordinate transformations on M, while the gauge transformations applied to the fermionic mass matrix produce a new field, the Higgs scalar φ. For the example above, this field is precisely the isospin doublet, color singlet with hypercharge $-1/2$ of eqn [6]. Gauge transformations also apply to the ordinary Dirac operator, thereby producing the gauge fields A.

Dynamics The group of generalized coordinate transformations allowed us to construct the configuration space. In the almost commutative case it consists of Riemannian metrics, gauge fields, and Higgs scalars. We now want a dynamics on this configuration space. Of course, we want this dynamics to be invariant under the group of generalized coordinate transformations. Note that the spectrum of the Dirac operator is invariant under this group and Chamseddine and Connes (1997) define the spectral action as a regularized partition function of these eigenvalues.

On almost commutative geometries, the spectral action is equal to the Einstein–Hilbert action plus the Yang–Mills–Higgs ansatz (**Figure 2**). In other words, almost commutative geometry explains the forces mediated by gauge bosons and Higgs scalars as pseudoforces accompanying the gravitational force in the same way that Minkowskian geometry (i.e., special relativity) explains the magnetic force as a pseudoforce accompanying the electric force.

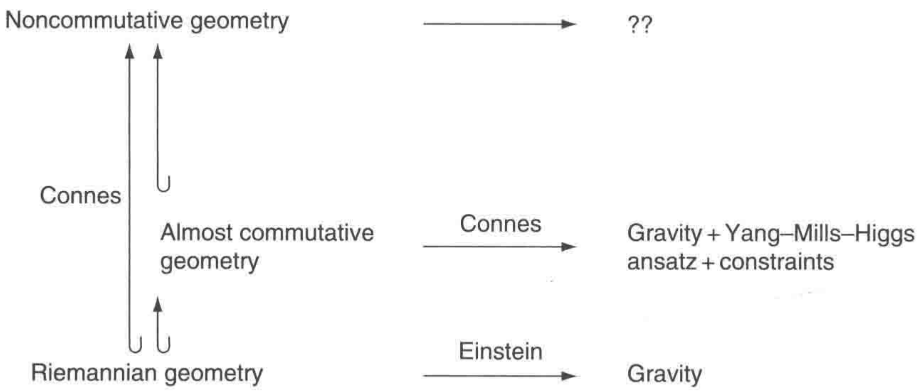


Figure 2 Deriving the Yang–Mills–Higgs ansatz from gravity.

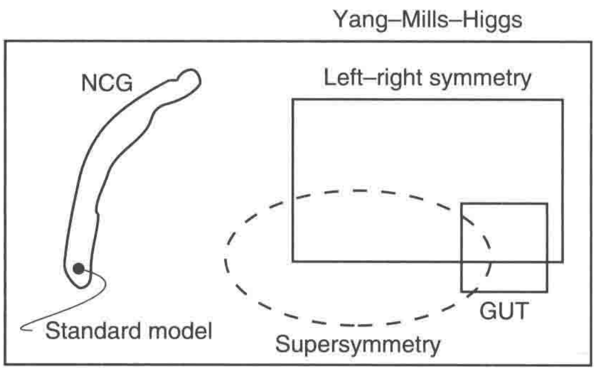


Figure 3 Constraints inside the ansatz.

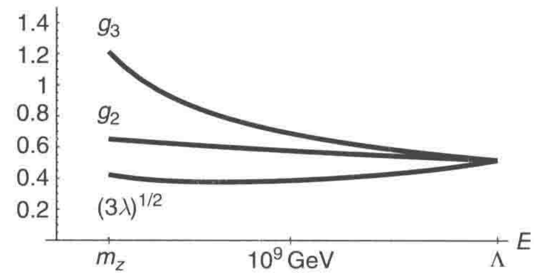


Figure 4 Running coupling constants.

There are constraints on the discrete and continuous parameters in the Yang–Mills–Higgs ansatz deriving from the spectral action **Figure 3**.

In particular, if we consider only irreducible spectral triples and among them only those which produce nondegenerate fermion masses compatible with renormalization, then we only get the standard model with one generation of quarks and leptons, with a massless neutrino and with an arbitrary number of colors, and a few submodels thereof. More than one generation and neutrino masses are possible but imply reducible triples. However, in at least one generation, the neutrino must remain purely left and massless.

For the standard model with N generations and N_c colors, we have the constraints $g_{N_c}^2 = g_2^2 = (9/N)\lambda$ on the continuous parameters. If we put $N = N_c = 3$ and if we believe in the popular "big desert" then these constraints yield a "unification scale" $\Lambda = 10^{17}$ GeV at which the uncertainty relation in spacetime should become manifest, $\Delta\tau = \hbar/\Lambda$, and a Higgs mass of $m_\varphi = 171.6 \pm 5$ GeV for $m_t = 174.3 \pm 5.1$ GeV (see **Figure 4**).

It is clear that almost commutative geometries only scratch the surface of a gold mine. May we hope that a genuinely noncommutative geometry will solve our present problems with quantum field theory and quantum gravity?

See also: Compact Groups and Their Representations; Dirac Fields in Gravitation and Nonabelian Gauge Theory; Effective Field Theories; General Relativity: Overview; Hopf Algebras and q-Deformation Quantum Groups; Positive Maps on C^*-Algebras; Quantum Hall Effect; Standard Model of Particle Physics; Symmetries and Conservation Laws; Symmetry Breaking in Field Theory; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory.

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The Particle Data Group, *Particle Physics Booklet* and http://pdg.lbl.gov

Noncommutative Geometry from Strings

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Noncommutative Geometry from String Theory

The first use of noncommutative geometry in string theory appears in the work of Witten on open-string field theory where the noncommutativity is associated with the product of open-string fields. Noncommutative geometry appears in the recent development of string theory in the seminal work of Connes, Douglas, and Schwarz where they constructed and identified the compactification of Matrix theory on a noncommutative torus.

Matrix Theory Compactification and Noncommutative Geometry

The matrix theory (M-theory) is an 11-dimensional quantum theory of gravity which is believed to underlie all superstring theories. Banks, Fischler, Shenker, and Susskind proposed that the large N limit of the supersymmetric matrix quantum mechanics of N D0-branes should describe the M-theory compactified on a lightlike circle. Compactification of the M-theory on a torus can be easily achieved by considering the torus as the quotient space $\mathbb{R}^d/\mathbb{Z}^d$ with the quotient conditions

$$U_i^{-1}X^jU_i = X^j + \delta_i^j 2\pi R_i, \quad i = 1, \ldots, d \qquad [1]$$

Here R_i are the radii of the torus. The unitary translation generators U_i generate the torus. They satisfy $U_iU_j = U_jU_i$. T-dualizing the D0 brane system, eqn [1] leads to the dual description as a $(d+1)$-dimensional supersymmetric gauge theory on the dual toroidal D-brane. A noncommutative torus T_θ^d is defined by the modified relations

$$U_iU_j = e^{i\theta_{ij}}U_jU_i \qquad [2]$$

where θ_{ij} specify the noncommutativity. Compactification on a noncommutative torus can be easily accommodated and leads to noncommutative gauge theory on the dual D-brane. The parameters θ_{ij} can be identified with the components C_{-ij} of the 3-form potential in M-theory.

Since M-theory compactified on a circle leads to IIA string theory, the components C_{-ij} correspond to the Neveu–Schwarz (NS) B-field B_{ij} in IIA string theory. The physics of the D0 brane system in the presence of an NS B-field can also be studied from the viewpoint of IIA string theory. This led Douglas and Hull to obtain the same result that a noncommutative field theory lives on the D-brane. Toroidally compactified IIA string theory has a T-duality group $SO(d,d;\mathbb{Z})$. The T-duality symmetry gets translated into an equivalence relation between gauge theories on the noncommutative torus: a gauge theory on the noncommutative torus T_θ^d is equivalent to that on the noncommutative torus $T_{\theta'}^d$ if their noncommutativity parameters and metrics are related by a T-duality transformation. For example,

$$\theta' = (A\theta + B)(C\theta + D)^{-1}, \quad \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in SO(d,d;\mathbb{Z}) \qquad [3]$$

It is remarkable that the T-duality acts within the field theory level, rather than mixing up the field theory modes with the string winding states and other stringy excitations. Mathematically, eqn [3] is precisely the condition for the noncommutative tori T_θ^d and $T_{\theta'}^d$ to be Morita equivalent.

Open-String in *B*-Field

It was soon realized that the D-brane does not necessarily need to be toroidal in order to be noncommutative. A direct canonical quantization of the open-string system shows that a constant B-field on a D-brane leads to noncommutative geometry on the D-brane world volume. Consider an open string moving in a flat space with metric g_{ij} and a constant NS B-field. In the presence of a Dp brane, the components of the B-field not along the brane can be gauged away; thus, the B-field can

have effects only in the longitudinal directions along the brane. The world-sheet (bosonic) action for this part is

$$S = \frac{1}{4\pi\alpha'}\int_\Sigma d^2\sigma \times \left(g_{ij}\partial_a x^i \partial^a x^j - 2\pi\alpha' B_{ij}\epsilon^{ab}\partial_a x^i \partial_b x^j\right) \quad [4]$$

where $i, j = 0, 1, \ldots, p$ is along the brane. It is easy to see that the boundary condition $g_{ij}\partial_\sigma x^j + 2\pi i\alpha' B_{ij}\partial_\tau x^j = 0$ at $\sigma = 0, \pi$ is not compatible with the standard canonical quantization $[x^i(\tau,\sigma), x^j(\tau,\sigma')] = 0$ at the boundary. Taking the boundary condition as constraints and performing canonical quantization, one obtains the commutation relations

$$[a^i_m, a^j_n] = mG^{ij}\delta_{m+n}, \qquad [x^i_0, p^j_0] = iG^{ij}, \qquad [x^i_0, x^j_0] = i\theta^{ij} \quad [5]$$

Here, the open-string mode expansion is

$$x^i(\tau,\sigma) = x^i_0 + 2\alpha'(p^i_0\tau - 2\pi\alpha'(g^{-1}B)^i_j p^j_0\sigma) + \sqrt{2\alpha'}\sum_{n\neq 0}\frac{e^{-in\tau}}{n} \times \left(ia^i_n \cos n\sigma - 2\pi\alpha'(g^{-1}B)^i_j a^j_n \sin n\sigma\right)$$

G^{ij} and θ^{ij} are the symmetric and antisymmetric parts of the matrix $(g + 2\pi\alpha' B)^{-1ij}$:

$$G^{ij} = \left(\frac{1}{g + 2\pi\alpha' B}\, g\, \frac{1}{g - 2\pi\alpha' B}\right)^{ij}$$
$$\theta^{ij} = -(2\pi\alpha')^2\left(\frac{1}{g + 2\pi\alpha' B}\, B\, \frac{1}{g - 2\pi\alpha' B}\right)^{ij} \quad [6]$$

It follows from [5] that the boundary coordinates $x^i \equiv x^i(\tau, 0)$ obey the commutation relation

$$[x^i, x^j] = i\theta^{ij} \quad [7]$$

Relation [7] implies that the D-brane world volume, where the open-string endpoints live, is a noncommutative manifold. One may also start with the closed-string Green function and let its arguments to approach the boundary to obtain the open-string Green function

$$\langle x^i(\tau)x^j(\tau')\rangle = -\alpha' G^{ij}\ln(\tau - \tau')^2 + \frac{i}{2}\theta^{ij}\epsilon(\tau - \tau') \quad [8]$$

where $\epsilon(\tau)$ is the sign of τ. From [8], one can again extract the commutator [7]. $G_{ij} = g_{ij} - (2\pi\alpha')^2 (Bg^{-1}B)_{ij}$ is called the open-string metric since it controls the short-distance behavior of open strings. In contrast, the short-distance behavior for closed strings is controlled by the closed-string metric g_{ij}. One may also treat the boundary B-term in [4] as a perturbation to the open-string conformal field theory and from which one may extract [8] from the modified operator product expansion of the open-string vertex operators.

D-branes in the Wess–Zumino–Witten model provide another example of noncommutative geometry. In this case, the background is not flat since there is a nonzero $H = dB \sim k^{-1/2}$, where k is the level. Examining the vertex operator algebra, one obtains that D-branes are described by nonassociative deformations of fuzzy spheres with nonassociativity controlled by $1/k$.

String Amplitudes and Effective Action

The effect of the B-field on the open-string amplitudes is simple to determine since only the x^i_0 commutation relation is affected nontrivially. For example, the noncommutative gauge theory can be obtained from the tree-level string amplitudes readily. For tree and one loop, the vertex operator formalism can be used. Generally, the vertex operator can be inserted at either the $\sigma = 0$ or $\sigma = \pi$ boundary, where the string has zero mode parts x^i_0 and $y^i_0 \equiv x^i_0 - (2\pi\alpha')^2(g^{-1}B)^i_j p^j_0$, respectively. The commutation relations are

$$[x^i_0, x^j_0] = i\theta^{ij}, \qquad [x^i_0, y^j_0] = 0, \qquad [y^i_0, y^j_0] = -i\theta^{ij} \quad [9]$$

The difference in the commutation relation for x_0 and y_0 implies that the two boundaries of the open string have opposite commutativity. This fact is not so important for tree-level calculations since one can always choose to put all the interactions at, for example, the $\sigma = 0$ boundary. Collecting all these zero mode parts of the vertex operators, one obtains a phase factor

$$e^{ip^1x_0}e^{ip^2x_0}\cdot e^{ip^Nx_0} = e^{i\sum p^a x_0}e^{-(i/2)\sum_{I<J}^N p^I\theta p^J} \quad [10]$$

where the external momenta p^a are ordered cyclically on the circle, and momentum conservation has been used. The computation of the oscillator part of the amplitude is the same as in the $B = 0$ case, except that the metric G is employed in the contractions. As a result, the effect of the B-field on the tree-level string amplitude is simply to multiply the amplitude at $B = 0$ by the phase factor and to replace the metric by the metric G. A generic term in the tree-level effective action simply becomes

$$\int d^{p+1}x\sqrt{-\det g}\,\mathrm{tr}\,\partial^{n_1}\Phi_1\cdots\partial^{n_k}\Phi_k \to \int d^{p+1}x\sqrt{-\det G}\,\mathrm{tr}\,\partial^{n_1}\Phi_1 * \cdots * \partial^{n_k}\Phi_k \quad [11]$$

Here the star product, also called the Moyal product, is defined by

$$(f * g)(x) = \exp\left(\mathrm{i}\frac{\theta^{\mu\nu}}{2}\frac{\partial}{\partial x_1^\mu}\frac{\partial}{\partial x_2^\nu}\right) f(x_1)g(x_2)|_{x_1=x_2} \quad [12]$$

The star product is associative and noncommutative, and satisfies $\overline{f * g} = \bar{g} * \bar{f}$ under complex conjugation. Also, for functions that vanish rapidly enough at infinity, there holds

$$\int f * g = \int g * f = \int fg \quad [13]$$

An interesting consequence of the nonlocality as expressed by the noncommutative geometry [7] is the existence of a dipole excitation whose extent is proportional to its momentum, $\Delta x = k\theta$. This relation is at the heart of the "IR/UV mixing phenomenon" (see below) of noncommutative field theory.

At one- (and higher-) loop level, the different noncommutativities for the opposite boundaries of the open string become essential and give rise to new effects. In this case nonplanar diagrams require one to put vertex operators at the two different boundaries $\sigma = 0, \pi$. A more complicated phase factor, which involves internal as well as external momentum, results. This leads to IR/UV mixing in the noncommutative quantum field theory. The different noncommutativity for the opposite boundaries of the open string [9] is the basic reason for the IR/UV mixing in the noncommutative quantum field theory. The commutation relations [5] are valid at all loops; therefore, one can use them to construct the higher-loop string amplitudes from first principles. The effect of the B-field on the string interaction can easily be implemented into the Reggeon vertex and the complete higher loop amplitudes in the presence of the B-field have been constructed.

Low-Energy Limit – The Seiberg–Witten Limit and the NCOS Limit

The full open-string system is still quite complicated. One may try to decouple the infinite number of massive string modes to obtain a low-energy field-theoretic description by taking the limit $\alpha' \to 0$. Since open strings are sensitive to G and θ, one should take the limit such that G and θ are fixed. For the magnetic case $B_{0i} = 0$, Seiberg and Witten showed that this can be achieved with the following double scaling limit:

$$\alpha' \sim \epsilon^{1/2}, \quad g_{ij} \sim \epsilon \to 0 \quad [14]$$

with B_{ij} and everything else kept fixed. Assuming B is of rank r, then [6] becomes

$$G_{ij} = -(2\pi\alpha')^2 (Bg^{-1}B)_{ij}, \quad \theta^{ij} = (B^{-1})^{ij}, \quad \text{for } i,j = 1, \ldots, r \quad [15]$$

Otherwise $G_{ij} = g_{ij}, \theta^{ij} = 0$. One may also argue that the closed string decouples in this limit. As a result, in the low-energy limit a greatly simplified noncommutative Yang–Mills action $F * F$ is obtained (see below for more discussion of this field theory).

For the case of a constant electric field background, say $B_{01} \neq 0$, there is a critical electric field beyond which the open string becomes unstable and the theory does not make sense. Due to the presence of this upper bound of the electric field, one can show that there is no decoupling limit where one can reduce the string theory to a field theory on a noncommutative spacetime. However, one can consider a different scaling limit where one takes the closed-string metric scale to infinity appropriately as the electric field approaches the critical value. In this limit, all closed-string modes decouple. One obtains a novel noncritical string theory living on a noncommutative spacetime known as the noncommutative open string (NCOS).

Noncommutative Quantum Field Theory

Field theories on noncommutative spacetime are defined by using the star product instead of the ordinary product of the fields. To illustrate the general ideas, let us consider a single real scalar field theory with the action

$$S = \int \mathrm{d}^D x \left[\frac{1}{2}\partial_\mu\phi * \partial^\mu\phi - \frac{m^2}{2}\phi * \phi - V(\phi)\right]$$
$$V(\phi) = \frac{g}{4!}\phi^{*4} \quad [16]$$

Due to the property [13], free noncommutative field theory is the same as an ordinary field theory. Treating the interaction term as a perturbation, one can perform the usual quantization and obtain the Feynman rules: the propagator is unchanged and the interaction vertex in the momentum space is given by g times the phase factor

$$\exp\left(-\frac{\mathrm{i}}{2}\sum_{1\le a<b\le 4} p^a \times p^b\right) \quad [17]$$

Here $p \times q \equiv p_\mu \theta^{\mu\nu} q_\nu$. The theory is nonlocal due to the infinite order of derivatives that appear in the interaction.

Planar and Nonplanar Diagrams

The factor [17] is cyclically symmetric but not permutation symmetric. This is analogous to the situation of an M-field theory. Using the same double-line notation as introduced by 't Hooft, one can similarly classify the Feynman diagrams of noncommutative field theory according to its genus. In particular, the total phase factor of a planar diagram behaves quite differently from that of a nonplanar diagram. It is easy to show that a planar diagram will have the phase factor

$$V_{\mathrm{p}}(p^1, \ldots, p^n) = \exp\left(-\frac{\mathrm{i}}{2} \sum_{1 \le a < b \le n} p^a \times p^b \right) \qquad [18]$$

where $p^1, \ldots, p^n$ are the (cyclically ordered) external momenta of the graph. Note that the phase factor [18] is independent of the internal momenta. This is not the case for a nonplanar diagram. One can easily show that a nonplanar diagram carries an additional phase factor

$$V_{\mathrm{np}} = V_{\mathrm{p}} \exp\left(-\frac{\mathrm{i}}{2} \sum_{1 \le a < b \le n} C_{ab} p^a \times p^b \right) \qquad [19]$$

where C_{ab} is the signed intersection matrix of the graph, whose ab matrix element counts the number of times the ath (internal or external) line crosses the bth line. The matrix C_{ab} is not uniquely determined by the diagram as different ways of drawing the graph could lead to different intersections. However, the phase factor [19] is unique due to momentum conservation.

The different behaviors of the planar and nonplanar phase factors have important consequences.

1. Since the phase factor [18] is independent of the internal momenta, the divergences and renormalizability of the planar diagrams will be (simply) the same as in the commutative theory and can be handled with standard renormalization techniques. This is sharply different for the nonplanar diagrams. In fact, due to the extra oscillatory internal-momenta-dependent phase factor, one can expect the nonplanar diagrams to have an improved ultraviolet (UV) behavior. It turns out that planar and nonplanar diagrams also differ sharply in their infrared (IR) behavior due to the "IR/UV mixing effect" (see below).
2. Moreover, at high energies one can expect that noncommutative field theory will generically become planar since the nonplanar diagrams will be suppressed due to the oscillatory phase factor.
3. In the limit $\theta \to \infty$, the nonplanar sector will be totally suppressed since the rapidly oscillating phase factor will cause the nonplanar diagram to vanish upon integrating out the momenta. Thus, generically the large θ limit is analogous to the large-N limit where only the planar diagrams contribute. However, these expectations do not apply for noncommutative gauge theory since one needs to include "open Wilson lines" (see below) in the construction of gauge invariant observables, and the open Wilson line grows in extent with energy and θ.

IR/UV Mixing

Due to the nonlocal nature of noncommutative field theory, there is generally a mixing of the UV and IR scales. The reason is roughly the following. Nonplanar diagrams generally have phase factors like $\exp(ik\theta p)$ with k a loop momentum, p an external momentum. Consider a nonplanar diagram which is UV divergent when $\theta = 0$; one can expect that for very high loop momenta the phase factor will oscillate rapidly and render the integral finite. However, this is only valid for a nonvanishing external momentum θp; the infinity will come back as $\theta p \to 0$. However, this time it appears as an IR singularity. Thus, an IR divergence arises whose origin is from the UV region of the momentum integration and this is known as the IR/UV mixing phenomenon.

To be more specific, consider the ϕ^4 scalar theory in $D = 4$ dimensions. The one-loop self-energy has a nonplanar contribution given by

$$\Gamma_{\mathrm{np}} = \frac{g}{6(2\pi)^4} \int \frac{\mathrm{d}^4 k}{k^2 + m^2} \mathrm{e}^{ik\theta p} \sim \frac{g}{3(4\pi^2)^2} \times (\Lambda_{\mathrm{eff}}^2 + \cdots) \qquad [20]$$

where $\Lambda_{\mathrm{eff}}^2 = (1/\Lambda^2 + (\theta p)^2)^{-1}$. One can see clearly the IR/UV mixing: Γ_{np} is UV finite as long as $\theta p \neq 0$; when $\theta p = 0$, the quadratic UV divergence is recovered, $\Gamma_{\mathrm{np}} \sim \Lambda^2$. For supersymmetric theory, one has at most logarithmic IR singularities from IR/UV mixing.

IR/UV mixing has a number of interesting consequences.

1. Due to the IR/UV mixing, noncommutative theory does not appear to have a consistent Wilsonian description since it requires that correlation functions computed at finite Λ differ from their limiting values by terms of order $1/\Lambda$ for all values of momenta. However, this is not true for theory with IR/UV mixing. For example, the two-point function [20] at finite value of Λ differs from its value at $\Lambda = \infty$ by the amount

$\Gamma^{\Lambda}_{\rm np} - \Gamma^{\Lambda=\infty}_{\rm np} \propto 1/(\theta p)^2$, for the range of momenta $(\theta p)^2 \ll 1/\Lambda^2$. It has been argued that the IR singularity may be associated with missing light degrees of freedom in the theory. With new degrees of freedom appropriately added, one may recover a conventional Wilsonian description. Moreover, it has been suggested to identify these degrees of freedom with the closed-string modes. However, the precise nature and origin of these degrees of freedom is not known.

2. The renormalization of the planar diagrams is straightforward; however, the situation is more subtle for the nonplanar diagrams since the IR/UV-mixed IR singularities may mix with other divergences at higher loops and render the proof of renormalizability much more difficult. IR/UV mixing renders certain large N noncommutative field theory nonrenormalizable. However, for theories with a fixed set of degrees of freedom to start with, it is believed that one can have sufficiently good control of the IR divergences and prove renormalizability. An example of renormalizable noncommutative quantum field theory is the noncommutative Wess–Zumino model where IR/UV mixing is absent. However, a general proof is still lacking.
3. One can show that IR/UV mixing in timelike noncommutative theory ($\theta^{0i} \neq 0$) leads to breakdown of perturbative unitarity. For a theory without IR/UV mixing, unitarity will be respected even if the theory has a timelike noncommutativity. Theory with lightlike noncommutativity is unitary.

Noncommutative Gauge Theory

Gauge theory on noncommutative space is defined by the action

$$S = -\frac{1}{4g^2}\int \mathrm{d}x\, \mathrm{tr}\big(F_{ij}(x) * F^{ij}(x)\big) \qquad [21]$$

where the gauge fields A_i are $N \times N$ Hermitian matrices, F_{ij} is the noncommutative field strength $F_{ij} = \partial_i A_j - \partial_j A_i - \mathrm{i}[A_i, A_j]_*$, and tr is the ordinary trace over $N \times N$ matrices. The theory is invariant under the star-gauge transformation

$$A_i \to g * A_i * g^\dagger - \mathrm{i}g * \partial_i g^\dagger \qquad [22]$$

where the $N \times N$ matrix function $g(x)$ is unitary with respect to the star product $g * g^\dagger = g^\dagger * g = I$. The solution is $g = \mathrm{e}_*^{\mathrm{i}\lambda}$, where λ is Hermitian. In infinitesimal form, $\delta_\lambda A_i = \partial_i\lambda + \mathrm{i}[\lambda, A_i]_*$. The noncommutative gauge theory has N^2 Hermitian gauge fields. Because of the star product, the U(1) sector of the theory is not free and does not decouple from the SU(N) factor as in the commutative case. Note that this way of defining noncommutative gauge theory does not work for other Lie groups since the star commutator generally involves the commutator as well as the anticommutator of the Lie algebra; hence, the expressions above generally involve the enveloping algebra of the underlying Lie group. With the help of the "Seiberg–Witten map" (see below), one can construct an enveloping-algebra-valued gauge theory which has the same number of independent gauge fields and gauge parameters as the ordinary Lie-algebra-valued gauge theory. However, the quantum properties of these theories are much less understood. One may also introduce certain automorphisms in the noncommutative U(N) theory to restrict the dependence of the noncommutative space coordinates of the field configurations and obtain a notion of noncommutative theory with orthogonal and symplectic star-gauge group. However, the theory does not reduce to the standard gauge theory in the commutative limit $\theta \to 0$.

Open Wilson Line and Gauge-Invariant Observables

One remarkable feature of noncommutative gauge theory is the mixing of noncommutative gauge transformations and spacetime translations, as can be seen from the following identity:

$$\mathrm{e}^{\mathrm{i}kx} * f(x) * \mathrm{e}^{-\mathrm{i}kx} = f(x + k\theta) \qquad [23]$$

for any function f. This is analogous to the situation in general relativity where translations are also equivalent to gauge transformations (general coordinate transformations). Thus, as in general relativity, there are no local gauge-invariant observables in noncommutative gauge theory. The unification of spacetime and gauge fields in noncommutative gauge theory can also be seen from the fact that derivatives can be realized as commutators, $\partial_i f \to -\mathrm{i}[\theta^{-1}_{ij} x^j, f]$, and get absorbed into the vector potential in the covariant derivative

$$D_i = \partial_i + \mathrm{i}A_i \to -\mathrm{i}\theta^{-1}_{ij} x^j + \mathrm{i}A_i \qquad [24]$$

Equation [24] clearly demonstrates the unification of spacetime and gauge fields. Note that the field strength takes the form $F_{ij} = \mathrm{i}[D_i, D_j] + \theta^{-1}_{ij}$.

The Wilson line operator for a path C running from x_1 to x_2 is defined by

$$W(C) = P_* \exp\left(\mathrm{i}\int_C A\right) \qquad [25]$$

P_* denotes the path ordering with respect to the star product, with $A(x_2)$ at the right. It transforms as

$$W(C) \to g(x_1) * W(C) * g(x_2)^\dagger \qquad [26]$$

In commutative gauge theory, the Wilson line operator for closed loop (or its Fourier transform) is gauge invariant. In noncommutative gauge theory, the closed Wilson loops are no longer gauge invariant. Noncommutative generalization of the gauge invariant Wilson loop operator can be constructed most readily by deforming the Fourier transform of the Wilson loop operator. It turns out that the closed loop has to open in a specific way to form an open Wilson line in order to be gauge invariant. To see this, let us consider a path C connecting points x and $x + l$. Using [23], it is easy to see that the operator

$$\tilde{W}(k) \equiv \int \mathrm{d}x \, \mathrm{tr}\, W(C) * \mathrm{e}^{ikx}, \quad \text{with } l^j = k_i\theta^{ij} \qquad [27]$$

is gauge invariant. Just like Wilson loops in ordinary gauge theory, these operators also constitute an overcomplete set of gauge-invariant operators parametrized by the set of curves C. When $\theta = 0, C$ becomes a closed loop and we reobtain the (Fourier transformed) usual closed Wilson loop in commutative gauge theory. Noncommutative version of the loop equation for closed Wilson loop has been constructed and involves open Wilson line. The open Wilson line is instrumental in the construction of gauge-invariant observables. An important application is in the construction of various couplings of the noncommutative D-brane to the bulk supergravity fields. The equivalence of the commutative and noncommutative couplings to the RR fields leads to the exact expression for the Seiberg–Witten map. It is remarkable that the one-loop nonplanar effective action for noncommutative scalar theory, gauge theory, as well as the two-loop effective action for scalar can be written compactly in terms of open Wilson line. Based on this result, the physical origin of the IR/UV mixing has been elucidated. One may identify the open Wilson line with the dipole excitation generically presents in noncommutative field theory and hence explain the presence of the IR/UV mixing. IR/UV mixing may also be identified with the instability associated with the closed-string exchange of the noncommutative D-branes.

The Seiberg–Witten Map

The open string is coupled to the 1-form A_i living on the D-brane through the coupling $\int_{\partial\Sigma} A$. For slowly varying fields, the effective action for this gauge potential can be determined from the S-matrix and is given by the Dirac–Born–Infeld (DBI) action. In the presence of a B-field, the discussion above (see eqn [11]) leads to the noncommutative DBI Lagrangian

$$L_{\mathrm{NCDBI}}(\hat{F}) = G_s^{-1}\mu_p\sqrt{-\det(G + 2\pi\alpha'\hat{F})} \qquad [28]$$

where $\mu_p = (2\pi)^{-p}(\alpha')^{-(p+1)/2}$ is the D-brane tension and $\hat{F}$ is the noncommutative field strength. However, one may also exploit the tensor gauge invariance on the D-brane (i.e., the string sigma model is invariant under $A \to A - \Lambda, B \to B + \mathrm{d}\Lambda$) and consider the combination $F + B$ as a whole. In this case, it is like having the open string coupled to the boundary gauge field strength $F + B$ and there is no B field. One has the usual DBI Lagrangian

$$L_{\mathrm{DBI}}(F) = g_s^{-1}\mu_p\sqrt{-\det(G + 2\pi\alpha'(F + B))} \qquad [29]$$

In [28] and [29], G_s and g_s are the effective open-string couplings in the noncommutative and commutative descriptions. Although they look quite different, Seiberg and Witten showed that the commutative and noncommutative DBI actions are indeed equivalent if the open-string couplings are related by $g_s = G_s\sqrt{\det(g + 2\pi\alpha' B)/\det G}$ and there is a field redefinition that relates the commutative and noncommutative gauge fields. The map $\hat{A} = \hat{A}(A)$ is called the Seiberg–Witten map. Moreover, the noncommutative gauge symmetry is equivalent to the ordinary gauge symmetry in the sense that they have the same set of orbits under gauge transformation:

$$\hat{A}(A) + \hat{\delta}_{\hat{\lambda}}\hat{A}(A) = \hat{A}(A + \delta_\lambda A) \qquad [30]$$

Here $\hat{A}_i$ and $\hat{\lambda}$ are, respectively, the noncommutative gauge field and noncommutative gauge transformation parameter, and A_i and λ are, respectively, the ordinary gauge field and ordinary transformation parameter. The map between $\hat{A}_i$ and A_i is called the Seiberg–Witten map. Equation [30] can be solved only if the transformation parameter $\hat{\lambda} = \hat{\lambda}(\lambda, A)$ is field dependent. The Seiberg–Witten map is characterized by the Seiberg–Witten differential equation

$$\delta\hat{A}_i(\theta) = \tfrac{1}{4}\delta\theta^{kl}\Big[\hat{A}_k * (\partial_l\hat{A}_i + \hat{F}_{li}) + (\partial_l\hat{A}_i + \hat{F}_{li}) * \hat{A}_k\Big] \qquad [31]$$

An exact solution for the Seiberg–Witten map can be written down with the help of the open Wilson

line. For the case of U(1) with constant F, we have the exact solution $\hat{F} = (1 + F\theta)^{-1}F$.

That there is a field redefinition that allows one to write the effective action in terms of different fields with different gauge symmetries may seem puzzling at first sight. However, it has a clear physical origin in terms of the string world sheet. In fact, there are different possible schemes to regularize the short-distance divergence on the world sheet. One can show that the Pauli–Villars regularization gives the commutative description, while the point-splitting regularization gives the noncommutative description. Since theories defined by different regularization schemes are related by a coupling-constant redefinition, this implies that the commutative and noncommutative descriptions are related by a field redefinition, because the couplings on the world sheet are just the spacetime fields.

Despite this formal equivalence, the physics of the noncommutative theories is generally quite different from the commutative case. First, it is clear that generally the Seiberg–Witten map may take nonsingular configurations to singular configurations. Second, the observables one is interested in are also generally different. Moreover, the two descriptions are generally good for different regimes: the conventional gauge theory description is simpler for small B and the noncommutative description is simpler for large B.

Perturbative Gauge Theory Dynamics

The noncommutative gauge symmetry [22] can be fixed as usual by employing the Faddeev–Popov procedure, resulting in Feynman rules that are similar to the conventional gauge theory. The important difference is that now the structure constants in the phase factors [18] and [19] should be amended. It turns out that the nonplanar U(N) diagrams contribute (only) to the U(1) part of the theory. As a result, unlike the commutative case, the U(1) part of the theory is no longer decoupled and free. Noncommutative gauge theory is one-loop renormalizable. The β-function is determined solely by the planar diagrams and, at one loop, is given by

$$\beta(g) = -\frac{22}{3}\frac{Ng^3}{16\pi^2} \quad \text{for } N \geq 1 \qquad [32]$$

Note that the β-function is independent of θ; the noncommutative U(1) is asymptotically free and does not reduce to the commutative theory when $\theta \to 0$. Noncommutative theory beyond the tree level is generally not smooth in the limit $\theta \to 0$. Discontinuity of this kind was also noted for the Chern–Simon system.

Gauge anomalies can be similarly discussed and satisfy the noncommutative generalizations of the Wess–Zumino consistency conditions. In $d = 2n$ dimensions, the anomaly involves the combination $\mathrm{tr}(T^{a_1}T^{a_2}\cdots T^{a_{n+1}})$ rather than the usual symmetrized trace, since the phase factor is not permutation symmetric. As a result, the usual cancellation of the anomaly does not work and is the main obstacle to the construction of noncommutative chiral gauge theory.

There are a number of interesting features to mention for the IR/UV mixing in noncommutative gauge theory.

1. IR/UV mixing generically yields pole-like IR singularities. Despite the appearance of IR poles, gauge invariance of the theory is not endangered.
2. One can show that only the U(1) sector is affected by IR/UV mixing.
3. As a result of IR/UV mixing, noncommutative U(1) photons polarized in the noncommutative plane will have different dispersion relations from those which are not. Strange as it is, this is consistent with gauge invariance.

Noncommutative Solitons, Instantons and D-Branes

Solitons and instantons play important roles in the nonperturbative aspects of field theory. The nonlocality of the star product gives noncommutative field theory a stringy nature. It is remarkable that this applies to the nonperturbative sector as well. Solitons and instantons in the noncommutative gauge theory amazingly reproduce the properties of D-branes in the string.

GMS Solitons

Derrick's theorem says that commutative scalar field theories in two or higher dimensions do not admit any finite-energy classical solution. This follows from a simple scaling argument, which will fail when the theory becomes noncommutative since noncommutativity introduces a fixed length scale $\sqrt{\theta}$. Noncommutative solitons in pure scalar theory can be easily constructed in the limit $\theta = \infty$. For example, consider a $(2+1)$-dimensional single scalar theory with a potential V and noncommutativity $\theta^{12} = \theta$. In the limit $\theta = \infty$, the potential term dominates and the noncommutative solitons are determined by the equation

$$\partial V/\partial\phi = 0 \qquad [33]$$

Equation [33] can be easily solved in terms of projectors. Assuming V has no linear term, the general soliton (up to unitary equivalence) is

$$\phi = \sum \lambda_i P_i \qquad [34]$$

where λ_i are the roots of $V'(\lambda) = 0$ and P_i is a set of orthogonal projectors. For real scalar field theory, the sum is restricted to real roots only. These solutions are known as the Gopakumar–Minwalla–Strominger (GMS) solitons. A simple example of a projector is given by $P = |0\rangle\langle 0|$, which corresponds to a Gaussian profile in the x^1, x^2 plane with width $\sqrt{\theta}$. The soliton continues to exist until θ decreases below a certain critical θ_c.

New solutions can be generated from known ones using the so-called solution-generating technique. If ϕ is a solution of [33], then

$$\phi' = T^\dagger \phi T \qquad [35]$$

is also a solution provided that $TT^\dagger = 1$. In an infinite-dimensional Hilbert space, T is not necessarily unitary, that is, $T^\dagger T \neq 1$. In this case, T is said to be a partial isometry. The new solution ϕ' is different from ϕ since they are not related by a global transformation of basis.

Tachyon Condensation and D-Branes

A beautiful application of the noncommutative soliton is in the construction of D-branes as solitons of the tachyon field in noncommutative open-string theory. For the bosonic string theory, one may consider it to be a space-filling D25 brane. Integrating out the massive-string modes leads to an effective action for the tachyon and the massless gauge field A_μ. It should be remarked that, contrary to the pure scalar case, noncommutative solitons can be constructed exactly for finite θ in a system with gauge and scalar fields. Although the detailed form of the effective action is unknown, one has enough confidence to say what the true vacuum configuration is according to the Sen conjecture. One can then apply the solution-generating technique to generate new soliton solutions. In this manner, with a B-field of rank $2k$, one can construct solutions which are localized in $\mathbb{R}^{2k}$ and represent a D$(25 - 2k)$ brane. This is supported by the matching of the tension and the spectrum of fluctuations around the soliton configuration. Similar ideas can also be applied to construct D-branes in type II string theory. Again the starting point is an unstable brane configuration with tachyon field(s). There are two types of unstable D-branes: non-BPS Dp branes (p odd in IIA theory and p even in IIB theory) and BPS branes–antibranes Dp–$\overline{\text{D}p}$ systems. A similar analysis allows one to identify the noncommutative soliton with the lower-dimensional BPS D-branes which arises from tachyon condensation.

One main motivation for studying tachyon condensation in open-string theory is the hope that open-string theory may provide a fundamental nonperturbative formulation of string theory. It may not be too surprising that D-branes can be obtained in terms of open-string fields. However, to describe closed strings and NS branes in terms of open-string degrees of freedom remains an obstacle.

Noncommutative Instanton and Monopoles

Instantons on noncommutative $\mathbb{R}^4_\theta$ can be readily constructed using the Atiyah–Drinfeld–Hitchin–Manin (ADHM) formalism by modifying the ADHM constraints with a constant additive term. The result is that the self-dual (resp. anti-self-dual) instanton moduli space depends only on the anti-self-dual (resp. self-dual) part. The construction goes through even in the U(1) case. Consider a self-dual θ; the ADHM constraints for the self-dual instanton are the same as in the commutative case, and there is no nonsingular solution. On the other hand, the ADHM constraints for the anti-self-dual instanton get modified and admit nontrivial solutions. This noncommutative instanton solution is nonsingular with size $\sqrt{\theta}$. The noncommutative instanton represents a D(p–4) brane within a Dp brane. The ADHM constraints are just the D-flatness condition for the D-brane world-volume gauge theory. The additive constant to the ADHM constraints also has a simple interpretation as a Fayet–Iliopolous parameter which appears in the presence of a B-field. Although the ADHM method does not give a self-dual instanton, a direct construction can be applied to obtain non-ADHM self-dual instantons. Recall that the gauge field strength can be written as $F_{ij} = \mathrm{i}[D_i, D_j] + \theta^{-1}_{ij}$, where D_i is given by the function on the right-hand side of [24]. Thus, a simple self-dual solution can be constructed with

$$D_i = \mathrm{i}\theta^{-1}_{ij} T^\dagger x^j T \qquad [36]$$

where T is a partial isometry which satisfies $TT^\dagger = 1$, but $T^\dagger T = 1 - P$ is not necessarily the identity. It is clear that P is a projector. The field strength

$$F_{ij} = \theta^{-1}_{ij} P \qquad [37]$$

is self-dual and has instanton number n where n is the rank of the projector.

On noncommutative $\mathbb{R}^3$ (say $\theta^{12} = \theta$), BPS monopoles satisfy the Bogomolny equation:

$$\nabla_i \Phi = \pm B_i, \quad i = 1, 2, 3 \qquad [38]$$

and can be obtained by solving the Nahm equation

$$\partial_z T_i = \epsilon_{ijk} T_j T_k + \delta_{i3}\theta \qquad [39]$$

T_i are $k \times k$ Hermitian matrices depending on an auxiliary variable z and k gives the charge of the monopole. Noncommutativity modifies the Nahm equation with a constant term, which can be absorbed by a constant shift of the generators. Therefore, unlike the case of instanton, the monopole moduli space is not modified by noncommutative deformation. The Nahm construction has a clear physical meaning in string theory. The monopole (electric charge) can be interpreted as a D-string (fundamental string) ending on a D3 brane. One can also suspend k D-string between a collection of N parallel D3 braness; this would correspond to a charge k monopole in a Higgsed U(N) gauge theory. The matrices X^i correspond to the matrix transverse coordinates of the D-strings which lie within the D3 branes.

Further Topics

Finally, in the following some further topics of interest are discussed briefly.

1. The noncommutative geometry discussed here is of canonical type. Other deformations exist, for example, kappa-deformation and fuzzy sphere which are of the Lie-algebra type, and quantum group deformation which is a quadratic-type deformation: $x^i x^j = q^{-1} \hat{R}^{ij}_{kl} x^k x^l$, whose consistency is guaranteed by the Yang–Baxter equation. It is interesting to see whether these noncommutative geometries arise from string theory. Another natural generalization is to consider noncommutative geometry of superspace. A simple example is to consider the fermionic coordinates to be deformed with the nonvanishing relation

$$\{\theta^\alpha, \theta^\beta\} = C^{\alpha\beta} \qquad [40]$$

   where $C^{\alpha\beta}$ are constants. It has been shown that [40] arises in certain Calabi–Yau compactification of type IIB string theory in the presence of RR background. The deformation [40] reduces the number of supersymmetries by half. Therefore, it is called $\mathcal{N} = 1/2$ supersymmetry. The noncommutativity [40] can be implemented on the superspace $(y^i, \theta^\alpha, \bar{\theta}^{\dot{\alpha}})$ as a star product for the θ^α's. Unlike the bosonic deformation which involves an infinite number of higher derivatives, the star product for [40] stops at order C^2 due to the Grassmannian nature of the fermionic coordinates. Field theory with $\mathcal{N} = 1/2$ supersymmetry is local and differs from the ordinary $\mathcal{N} = 1$ theory by only a small number of supersymmetry breaking terms. The $N = 1/2$ Wess–Zumino model is renormalizable if extra F and F^3 terms are added to the original Lagrangian, where F is the auxiliary field. The $N = 1/2$ gauge theory is also renormalizable.
2. Integrability of a theory provides valuable information beyond the perturbative level. An integrable field theory is characterized by an infinite number of conserved charges in involution. It is natural to ask whether integrability is preserved by noncommutative deformation. Noncommutative integrable field theories have been constructed. In the commutative case, Ward has conjectured that all $(1+1)$- and $(2+1)$-dimensional integrable systems can be obtained from the four-dimensional self-dual Yang–Mills equation by reduction. Validity of the noncommutative version of the Ward conjecture has been confirmed so far. It will be interesting to see whether it is true in general.
3. Locality and Lorentz symmetry form the cornerstones of quantum field theory and standard model physics of particles. Noncommutative field theory provides a theoretical framework where one can discuss effects of nonlocality and Lorentz symmetry violation. Possible phenomenological signals have been investigated (mostly at the tree level) and a bound has been placed on the extent of noncommutativity. A proper understanding and better control of the IR/UV mixing remains the crux of the problem. Noncommutative geometry may also be relevant for cosmology and inflation.
4. Like the standard AdS/CFT correspondence, the noncommutative gauge theory should also have a gravity-dual description. The supergravity background can be determined by considering the decoupling limit of D-branes with an NS B-field background. However, since the noncommutative gauge theory does not permit any conventional local gauge-invariant observable, the usual AdS/CFT correspondence that relates field theory correlators with bulk interaction does not seem to apply. It has been argued that generic properties such as the relation between length and momentum for open Wilson lines

can be seen from the gravity side. A more precise understanding of the duality map is called for.

See also: Brane Construction of Gauge Theories; Deformation Quantization; Gauge Theories from Strings; Noncommutative Tori, Yang–Mills, and String Theory; Positive Maps on C^*-Algebras; Solitons and Other Extended Field Configurations; String Field Theory; Superstring Theories.

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Noncommutative Tori, Yang–Mills, and String Theory

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Introduction

Noncommutative tori are historically among the oldest and by now the most developed examples of noncommutative spaces. Noncommutative Yang–Mills theory can be obtained from string theory. This connection led to a cross-fertilization of research in physics and mathematics on Yang–Mills theory on noncommutative tori. One important result stemming from that work is the link between T-duality in string theory and Morita equivalence of associative algebras. In this article, we give an overview of the basic results in the differential geometry of noncommutative tori. Yang–Mills theory on noncommutative tori, the duality induced by Morita equivalence and its link with T-duality are discussed. The noncommutative Nahm transform for instantons is introduced.

Noncommutative Tori

The Algebra of Functions

The basic notions of noncommutative differential geometry were introduced and illustrated on the example of a two-dimensional noncommutative torus by Connes (1980). To define an algebra of functions on a d-dimensional noncommutative torus, consider a set of linear generators $U_{\boldsymbol{n}}$ labeled by $\boldsymbol{n} \in \mathbb{Z}^d$ – a d-dimensional vector with integral entries. The multiplication is defined by the formula

$$U_{\boldsymbol{n}} U_{\boldsymbol{m}} = e^{\pi i n_j \theta^{jk} m_k} U_{\boldsymbol{n}+\boldsymbol{m}} \qquad [1]$$

where θ^{jk} is an antisymmetric $d \times d$ matrix, and summation over repeated indices is assumed. We further extend the multiplication from finite linear combinations to formal infinite series $\sum_{\boldsymbol{n}} C(\boldsymbol{n}) U_{\boldsymbol{n}}$ where the coefficients $C(\boldsymbol{n})$ tend to zero faster than any power of $\|\boldsymbol{n}\|$. The resulting algebra constitutes the algebra of smooth functions on a noncommutative torus and will be denoted by T_θ^d. Sometimes for brevity we will omit the dimension label d in the notation of the algebra. We introduce an involution $*$ in T_θ^d by the rule $U_{\boldsymbol{n}}^* = U_{-\boldsymbol{n}}$. The elements $U_{\boldsymbol{n}}$ are assumed to be unitary with respect to this involution, that is, $U_{\boldsymbol{n}}^* U_{\boldsymbol{n}} = U_{-\boldsymbol{n}} U_{\boldsymbol{n}} = 1 \equiv U_0$. One can further introduce a norm and take an appropriate completion of the involutive algebra T_θ^d to obtain the C^*-algebra of functions on a noncommutative torus. For our purposes, the norm structure will not be important. A canonically normalized trace on T_θ^d is introduced by specifying

$$\mathrm{tr}\, U_{\boldsymbol{n}} = \delta_{\boldsymbol{n},0} \qquad [2]$$

Projective Modules

According to the general approach to noncommutative geometry, finitely generated projective modules

over the algebra of functions are natural analogs of vector bundles. Throughout this article, when speaking of a projective module, we will assume a finitely generated left projective module.

A free module $(T^d_\theta)^N$ is equipped with a T^d_θ-valued Hermitian inner product $\langle .,. \rangle_{T_\theta}$ defined by the formula

$$\langle (a_1,\ldots,a_N),(b_1,\ldots,b_N)\rangle_{T_\theta} = \sum_{i=1}^{N} a_i^* b_i \qquad [3]$$

A projective module E is by definition a direct summand of a free module. Thus, it inherits the inner product $\langle .,. \rangle_{T_\theta}$. Consider the endomorphisms of the module E, that is, linear mappings $E \to E$ commuting with the action of T^d_θ. These endomorphisms form an associative unital algebra denoted $\mathrm{End}_{T_\theta} E$. A decomposition $(T^d_\theta)^N = E \oplus E'$ determines an endomorphism $P:(T^d_\theta)^N \to (T^d_\theta)^N$ that projects $(T^d_\theta)^N$ onto E. The algebra $\mathrm{End}_{T_\theta} E$ can then be identified with a subalgebra of $\mathrm{Mat}_N(T^d_{-\theta})$ – the endomorphisms of the free module $(T^d_\theta)^N$. The latter has a canonical trace that is the composition of the matrix trace with the trace specified in [2]. By restriction, it gives rise to a canonical trace tr on $\mathrm{End}_{T_\theta} E$. The same embedding also provides a canonical involution on $\mathrm{End}_{T_\theta} E$ by a composition of the matrix transposition and the involution $*$ on T^d_θ.

A large class of examples of projective modules over noncommutative tori are furnished by the so-called Heisenberg modules. They are constructed as follows. Let G be the direct sum of $\mathbb{R}^p$ and an abelian finitely generated group, and let G^* be its dual group. In the most general situation $G = \mathbb{R}^p \times \mathbb{Z}^q \times F$ where F is a finite group. Then $G^* \cong \mathbb{R}^p \times T^q \times F^*$.

Consider the linear space $\mathcal{S}(G)$ of functions on G decreasing at infinity faster than any power. We define operators $U_{(\gamma,\tilde{\gamma})}: \mathcal{S}(G) \to \mathcal{S}(G)$ labeled by a pair $(\gamma,\tilde{\gamma}) \in G \times G^*$ acting as follows:

$$(U_{(\gamma,\tilde{\gamma})} f)(x) = \tilde{\gamma}(x) f(x+\gamma) \qquad [4]$$

One can check that the operators $U_{(\gamma,\tilde{\gamma})}$ satisfy the commutation relations

$$U_{(\gamma,\tilde{\gamma})} U_{(\mu,\tilde{\mu})} = \tilde{\mu}(\gamma)\tilde{\gamma}^{-1}(\mu) U_{(\mu,\tilde{\mu})} U_{(\gamma,\tilde{\gamma})} \qquad [5]$$

If $(\gamma,\tilde{\gamma})$ run over a d-dimensional discrete subgroup $\Gamma \subset G \times G^*, \Gamma \cong \mathbb{Z}^d$, then formula [4] defines a module over a d-dimensional noncommutative torus T^d_θ with

$$\exp(2\pi \mathrm{i} \theta_{ij}) = \tilde{\gamma}_i(\gamma_j)\tilde{\gamma}_j^{-1}(\gamma_i) \qquad [6]$$

for a given basis $(\gamma_i,\tilde{\gamma}_i)$ of the lattice Γ. This module is projective if Γ is such that $G \times G^*/\Gamma$ is compact. If that is the case, then the projective T^d_θ-module at hand is called a Heisenberg module and denoted by E_Γ.

Heisenberg modules play a special role. If the matrix θ_{ij} is irrational in the sense that at least one of its entries is irrational, then any projective module over T^d_θ can be represented as a direct sum of Heisenberg modules. In that sense, Heisenberg modules can be used as building blocks to construct an arbitrary module.

Connections

Next we would like to define connections on a projective module over T^d_θ. To this end, let us first define a Lie algebra of shifts L_θ acting on T^d_θ by specifying a basis consisting of derivations $\delta_j : T^d_\theta \to T^d_\theta, j = 1,\ldots,d$ satisfying

$$\delta_j(U_{\boldsymbol{n}}) = 2\pi \mathrm{i} n_j U_{\boldsymbol{n}} \qquad [7]$$

These derivations span a d-dimensional abelian Lie algebra that we denote by L_θ.

A connection on a module E over T^d_θ is a set of operators $\nabla_X : E \to E, X \in L_\theta$, depending linearly on X and satisfying

$$[\nabla_X, U_{\boldsymbol{n}}] = \delta_X(U_{\boldsymbol{n}}) \qquad [8]$$

where $U_{\boldsymbol{n}}$ are operators $E \to E$ representing the corresponding generators of T^d_θ. In the standard basis [7], this relation reads as

$$[\nabla_j, U_{\boldsymbol{n}}] = 2\pi \mathrm{i} n_j U_{\boldsymbol{n}} \qquad [9]$$

The curvature of the connection ∇_X defined as the commutator $F_{XY} = [\nabla_X, \nabla_Y]$ is an exterior 2-form on the adjoint vector space L^*_θ with values in $\mathrm{End}_{T^d_\theta} E$.

K-Theory: Chern Character

The K-groups of a noncommutative torus coincide with those for commutative tori:

$$K_0(T^d_\theta) \cong \mathbb{Z}^{2^{d-1}} \cong K_1\left(T^d_\theta\right)$$

The Chern character of a projective module E over a noncommutative torus T^d_θ can be defined as

$$\mathrm{ch}(E) = \mathrm{tr}\, \exp\left(\frac{F}{2\pi \mathrm{i}}\right) \in \Lambda^{\mathrm{even}}(L^*_\theta) \qquad [10]$$

where F is the curvature form of a connection on E, $\Lambda^{\mathrm{even}}(L^*_\theta)$ is the even part of the exterior algebra of L^*_θ and tr is the canonical trace on $\mathrm{End}_{T^d_\theta} E$. This

mapping gives rise to a noncommutative Chern character

$$\mathrm{ch}: K_0\left(T_\theta^d\right) \to \Lambda^{\mathrm{even}}\left(L_\theta^*\right) \qquad [11]$$

The component $\mathrm{ch}_0(E) = \mathrm{tr}\, \mathbf{1} \equiv \dim(E)$ is called the dimension of the module E.

A distinctive feature of the noncommutative Chern character [11] is that its image does not consist of integral elements, that is, there is no lattice in L_θ^* that generates the image of the Chern character. However, there is a different integrality statement that replaces the commutative one. Consider a basis in L_θ^* in which the derivations corresponding to basis elements satisfy [7]. Denote the exterior forms corresponding to the basis elements by $\alpha^1, \ldots, \alpha^d$. Then an arbitrary element of $\Lambda(L_\theta^*)$ can be represented as a polynomial in the anticommuting variables α^i. Next let us consider the subset $\Lambda^{\mathrm{even}}(\mathbb{Z}^d) \subset \Lambda^{\mathrm{even}}(L_\theta^*)$ that consists of polynomials in α^j having integer coefficients. It was proved by Elliott that the Chern character is injective and its range on $K_0(T_\theta^d)$ is given by the image of $\Lambda^{\mathrm{even}}(\mathbb{Z}^d)$ under the action of the operator

$$\exp\left(-\frac{1}{2}\frac{\partial}{\partial \alpha^j}\theta^{jk}\frac{\partial}{\partial \alpha^k}\right)$$

This fact implies that the K-group $K_0(T_\theta^d)$ can be identified with the additive group $\Lambda^{\mathrm{even}}(\mathbb{Z}^d)$.

The K-theory class $\mu(E) \in \Lambda^{\mathrm{even}}(\mathbb{Z}^d)$ of a module E can be computed from its Chern character by the formula

$$\mu(E) = \exp\left(\frac{1}{2}\frac{\partial}{\partial \alpha^j}\theta^{jk}\frac{\partial}{\partial \alpha^k}\right)\mathrm{ch}(E) \qquad [12]$$

Note that the anticommuting variables α^i and the derivatives $\partial/\partial\alpha^j$ satisfy the anticommutation relation $\{\alpha^i, \partial/\partial\alpha^j\} = \delta^i_j$.

The coefficients of $\mu(E)$ standing in front of monomials in α^i are integers to which we will refer as the topological numbers of the module E. These numbers can also be interpreted as numbers of D-branes of a definite kind although in noncommutative geometry it is difficult to talk about branes as geometrical objects wrapped on torus cycles.

One can show that for noncommutative tori T_θ^d with irrational matrix θ_{ij} the set of elements of $K_0(T_\theta^d)$ that represent a projective module (i.e., the positive cone) consist exactly of the elements of positive dimension. Moreover, if θ_{ij} is irrational, any two projective modules which represent the same element of $K_0(T_\theta^d)$ are isomorphic; that is, the projective modules are essentially specified in this case by their topological numbers.

The complex differential geometry of noncommutative tori and its relation with mirror symmetry is discussed in Polishchuk and Schwarz (2003).

Yang–Mills Theory on Noncommutative Tori

Let E be a projective module over T_θ^d. We call a Yang–Mills field on E a connection ∇_X-compatible with the Hermitian structure, that is, a connection satisfying

$$\langle \nabla_X \xi, \eta \rangle_{T_\theta} + \langle \xi, \nabla_X \eta \rangle_{T_\theta} = \delta_X(\langle \xi, \eta \rangle_{T_\theta}) \qquad [13]$$

for any two elements $\xi, \eta \in E$. Given a positive-definite metric on the Lie algebra L_θ, we can define a Yang–Mills functional

$$S_{\mathrm{YM}}(\nabla_i) = \frac{V}{4g_{\mathrm{YM}}^2} g^{ik} g^{jl} \mathrm{tr}(F_{ij} F_{kl}) \qquad [14]$$

Here g^{ij} stands for the metric tensor in the canonical basis [7], $V = \sqrt{|\det g|}$, g_{YM} is the Yang–Mills coupling constant, tr stands for the canonical trace on $\mathrm{End}_{T_\theta} E$ discussed above, and summation over repeated indices is assumed. Compatibility with the Hermitian structure [13] can be shown to imply the positive definiteness of the functional S_{YM}. The extrema of this functional are given by the solutions to the Yang–Mills equations

$$g^{ki}[\nabla_k, F_{ij}] = 0 \qquad [15]$$

A gauge transformation in the noncommutative Yang–Mills theory is specified by a unitary endomorphism $Z \in \mathrm{End}_{T_\theta} E$, that is, an endomorphism satisfying $ZZ^* = Z^*Z = 1$. The corresponding gauge transformation acts on a Yang–Mills field as

$$\nabla_j \mapsto Z \nabla_j Z^* \qquad [16]$$

The Yang–Mills functional [14] and the Yang–Mills equations [15] are invariant under these transformations.

It is easy to see that Yang–Mills fields whose curvature is a scalar operator, that is, $[\nabla_i, \nabla_j] = \sigma_{ij} \cdot \mathbf{1}$ with σ_{ij} a real-number-valued tensor, solve the Yang–Mills equations [15]. A characterization of modules admitting a constant curvature connection and a description of the moduli spaces of constant curvature connections (i.e., the space of such connections modulo gauge transformations) is reviewed in Konechny and Schwarz (2002). Another interesting class of solutions to the Yang–Mills equations is instantons (see below).

As in the ordinary field theory, one can construct various extensions of the noncommutative Yang–Mills theory [14] by adding other fields. To obtain a

supersymmetric extension of [14], one needs to add a number of endomorphisms $X_I \in \mathrm{End}_{T_\theta}E$ that play the role of bosonic scalar fields in the adjoint representation of the gauge group and a number of odd Grassmann parity endomorphisms $\psi_i^\alpha \in \Pi\mathrm{End}_{T_\theta}E$ endowed with an SO(d)-spinor index α. The latter ones are analogs of the usual fermionic fields.

In string theory, one considers a maximally supersymmetric extension of the Yang–Mills theory [14]. In this case, the supersymmetric action depends on $10-d$ bosonic scalars $X_I, I=d,\ldots,9$, and the fermionic fields can be collected into an SO(9, 1) Majorana–Weyl spinor multiplet $\psi^\alpha, \alpha=1,\ldots,16$. The maximally supersymmetric Yang–Mills action takes the form

$$S_{\mathrm{SYM}} = \frac{V}{4g^2}\mathrm{tr}\Big(F_{\mu\nu}F^{\mu\nu} + [\nabla_\mu, X_I][\nabla^\mu, X^I] + [X_I, X_J][X^I, X^J] - 2\psi^\alpha\sigma^\mu_{\alpha\beta}[\nabla_\mu, \psi^\beta] - 2\psi^\alpha\sigma^I_{\alpha\beta}[X_I, \psi^\beta]\Big) \qquad [17]$$

Here the curvature indices $F_{\mu\nu}, \mu,\nu=0,\ldots,d-1$, are assumed to be contracted with a Minkowski signature metric, and $\sigma^A_{\alpha\beta}$ are blocks of the ten-dimensional 32×32 gamma-matrices

$$\Gamma_A = \begin{pmatrix} 0 & \sigma_A^{\alpha\beta} \\ (\sigma_A)_{\alpha\beta} & 0 \end{pmatrix}, \quad A=0,\ldots,9$$

This action is invariant under two kinds of supersymmetry transformations denoted by $\delta_\epsilon, \tilde{\delta}_\epsilon$ and defined as

$$\begin{aligned} &\delta_\epsilon\psi = \tfrac{1}{2}(\sigma^{jk}F_{jk}\epsilon + \sigma^{jI}[\nabla_j, X_I]\epsilon + \sigma^{IJ}[X_I, X_J]\epsilon) \\ &\delta_\epsilon\nabla_j = \epsilon\sigma_j\psi, \quad \delta_\epsilon X_J = \epsilon\sigma_J\psi \\ &\tilde{\delta}_\epsilon\psi = \epsilon, \quad \tilde{\delta}_\epsilon\nabla_j = 0, \quad \tilde{\delta}_\epsilon X_J = 0 \end{aligned} \qquad [18]$$

where ϵ is a constant 16-component Majorana–Weyl spinor. Of particular interest for string theory applications are solutions to the equations of motion corresponding to [17] that are invariant under some of the above supersymmetry transformations. Further discussion can be found in Konechny and Schwarz (2002).

Morita Equivalence

The role of Morita equivalence as a duality transformation in noncommutative Yang–Mills theory was elucidated by Schwarz (1998). We will adopt a definition of Morita equivalence for noncommutative tori which can be shown to be essentially equivalent to the standard definition of strong Morita equivalence. We will say that two noncommutative tori T^d_θ and $T^d_{\hat\theta}$ are Morita equivalent if there exists a $(T^d_\theta, T^d_{\hat\theta})$-bimodule Q and a $(T^d_{\hat\theta}, T^d_\theta)$-bimodule P such that

$$Q \otimes_{T_{\hat\theta}} P \cong T_\theta, \qquad P \otimes_{T_\theta} Q \cong T_{\hat\theta} \qquad [19]$$

where T_θ on the right-hand side is considered as a (T_θ, T_θ)-bimodule and analogously for $T_{\hat\theta}$. (It is assumed that the isomorphisms are canonical.) Given a T_θ-module E one obtains a $T_{\hat\theta}$-module $\hat{E}$ as

$$\hat{E} = P \otimes_{T_\theta} E \qquad [20]$$

One can show that this mapping is functorial. Moreover, the bimodule Q provides us with an inverse mapping $Q \otimes_{T_{\hat\theta}} \hat{E} \cong E$.

We further introduce a notion of gauge Morita equivalence (originally called "complete Morita equivalence") that allows one to transport connections along with the mapping of modules [20]. Let L be a d-dimensional commutative Lie algebra. We say that the $(T^d_{\hat\theta}, T^d_\theta)$ Morita equivalence bimodule P establishes a gauge Morita equivalence if it is endowed with operators $\nabla^P_X, X \in L$ that determine a constant curvature connection simultaneously with respect to T^d_θ and $T^d_{\hat\theta}$, that is, satisfy

$$\begin{aligned} &\nabla^P_X(ea) = (\nabla^P_X e)a + e(\delta_X a) \\ &\nabla^P_X(\hat{a}e) = \hat{a}(\nabla^P_X e) + (\hat{\delta}_X\hat{a})e \\ &[\nabla^P_X, \nabla^P_Y] = 2\pi i\sigma_{XY}\cdot \mathbf{1} \end{aligned} \qquad [21]$$

Here δ_X and $\hat{\delta}_X$ are standard derivations on T_θ and $T_{\hat\theta}$, respectively. In other words, we have two Lie algebra homomorphisms

$$\delta : L \to L_\theta, \qquad \hat{\delta} : L \to L_{\hat\theta} \qquad [22]$$

If a pair (P, ∇^P_X) specifies a gauge $(T_\theta, T_{\hat\theta})$-equivalence bimodule, then there exists a correspondence between connections on E and connections on $\hat{E}$. The connection $\hat{\nabla}_X$ on $\hat{E}$ corresponding to a given connection ∇_X on E is defined as

$$\nabla_X \mapsto \hat{\nabla}_X = 1 \otimes \nabla_X + \nabla^P_X \otimes 1 \qquad [23]$$

More precisely, an operator $1\otimes\nabla_X + \nabla^P_X \otimes 1$ on $P \otimes_{\mathbb{C}} E$ descends to a connection $\hat{\nabla}_X$ on $\hat{E} = P\otimes_{T_\theta} E$. It is straightforward to check that under this mapping gauge equivalent connections go to gauge equivalent ones,

$$Z^\dagger \nabla_X Z = \hat{Z}^\dagger \hat{\nabla}_X \hat{Z}$$

where $\hat{Z} = 1 \otimes Z$ is the endomorphism of $\hat{E} = P \otimes_{T_\theta} E$ corresponding to $Z \in \mathrm{End}_{T^d_\theta} E$.

The curvatures of $\hat{\nabla}_X$ and ∇_X are connected by the formula

$$F^{\nabla}_{XY} = \hat{F}^{\nabla}_{XY} + \mathbf{1}\sigma_{XY} \quad [24]$$

which in particular shows that constant curvature connections go to constant curvature ones.

Since noncommutative tori are labeled by an antisymmetric $d \times d$ matrix θ, gauge Morita equivalence establishes an equivalence relation on the set of such matrices. To describe this equivalence relation, consider the action $\theta \mapsto h\theta = \hat{\theta}$ of $SO(d, d|\mathbb{Z})$ on the space of antisymmetric $d \times d$ matrices by the formula

$$\hat{\theta} = (M\theta + N)(R\theta + S)^{-1} \quad [25]$$

where the $d \times d$ matrices M, N, R, S are such that the matrix

$$h = \begin{pmatrix} M & N \\ R & S \end{pmatrix} \quad [26]$$

belongs to the group $SO(d, d|\mathbb{Z})$. The above action is defined whenever the matrix $A \equiv R\theta + S$ is invertible. One can prove that two noncommutative tori T^d_θ and $T_{\hat{\theta}}$ are gauge Morita equivalent if and only if the matrices θ and $\hat{\theta}$ belong to the same orbit of the $SO(d, d|\mathbb{Z})$ action [25].

The duality group $SO(d, d|\mathbb{Z})$ also acts on the topological numbers of moduli $\mu \in \Lambda^{\text{even}}(\mathbb{Z}^d)$. This action can be shown to be given by a spinor representation constructed as follows. First note that the operators $a^i = \alpha^i, b_i = \partial/\partial\alpha^i$ act on $\Lambda(\mathbb{R}^d)$ and give a representation of the Clifford algebra specified by the metric with signature (d, d). The group $O(d, d|\mathbb{C})$ can thus be regarded as a group of automorphisms acting on the Clifford algebra generated by a^i, b_j. Denote the latter action by W_h for $h \in O(d, d|\mathbb{C})$. One defines a projective action V_h of $O(d, d|\mathbb{C})$ on $\Lambda(\mathbb{R}^d)$ according to

$$V_h a^i V_h^{-1} = W_{h^{-1}}(a^i), \qquad V_h b_j V_h^{-1} = W_{h^{-1}}(b_j)$$

This projective action can be restricted to yield a double-valued spinor representation of $SO(d, d|\mathbb{C})$ on $\Lambda(\mathbb{R}^d)$ by choosing a suitable bilinear form on $\Lambda(\mathbb{R}^d)$. The restriction of this representation to the subgroup $SO(d, d|\mathbb{Z})$ acting on $\Lambda^{\text{even}}(\mathbb{Z}^d)$ gives the action of Morita equivalence on the topological numbers of moduli.

The mapping [23] preserves the Yang–Mills equations of motion [15]. Moreover, one can define a modification of the Yang–Mills action functional [14] in such a way that the values of the functionals on ∇_X and $\hat{\nabla}_X$ coincide up to an appropriate rescaling of coupling constants. The modified action functional has the form

$$S_{\text{YM}} = \frac{V}{4g^2}\operatorname{tr}(F_{jk} + \Phi_{jk} \cdot \mathbf{1})(F^{jk} + \Phi^{jk} \cdot \mathbf{1}) \quad [27]$$

where Φ^{jk} is a scalar-valued tensor that can be thought of as some background field. Adding this term will allow us to compensate for the curvature shift by adopting the transformation rule

$$\Phi_{XY} \mapsto \Phi_{XY} - \sigma_{XY}$$

Note that the new action functional [27] has the same equations of motion [15] as the original one.

To show that the functional [27] is invariant under gauge Morita equivalence, one has to take into account two more effects. Firstly, the values of trace change by a factor $c = \dim(\hat{E})(\dim(E))^{-1}$ as $\hat{\operatorname{tr}}\, \hat{X} = c \operatorname{tr} X$. Secondly, the identification of L_θ and $L_{\hat{\theta}}$ is established by means of some linear transformation A^k_j, the determinant of which will rescale the volume V. Both effects can be absorbed into an appropriate rescaling of the coupling constant.

One can show that the curvature tensor, the metric tensor, the background field Φ_{ij}, and the volume element V transform according to

$$\begin{aligned} F^{\hat{\nabla}}_{ij} &= A^k_i F^{\nabla}_{kl} A^l_j + \sigma_{ij} \\ \hat{g}_{ij} &= A^k_i g_{kl} A^l_j \\ \hat{\Phi}_{ij} &= A^k_i \Phi_{kl} A^l_j - \sigma_{ij} \\ \hat{V} &= V|\det A| \end{aligned} \quad [28]$$

where $A = R\theta + S$ and $\sigma = -RA^t$. The action functional [27] is invariant under the gauge Morita equivalence if the coupling constant transforms according to

$$\hat{g}^2_{\text{YM}} = g^2_{\text{YM}}|\det A|^{1/2} \quad [29]$$

Supersymmetric extensions of Yang–Mills theory on noncommutative tori were shown to arise within string theory essentially in two situations. In the first case, one considers compactifications of the (BFSS or IKKT) matrix model of M-theory (Connes *et al.* 1998). A discussion regarding the connection between T-duality and Morita equivalence in this case can be found in Seiberg and Witten (1999, section 7). Noncommutative gauge theories on tori can also be obtained by taking the so-called Seiberg–Witten zero slope limit in the presence of a Neveu–Schwarz B-field background (Seiberg and Witten 1999). The emergence of noncommutative geometry in this limit is discussed in this article. Below we give some details on the relation between T-duality and Morita equivalence in this approach. Consider a number of Dp-branes wrapped on T^p parametrized by

coordinates $x^i \sim x^i + 2\pi r$ with a closed-string metric G_{ij} and a B-field B_{ij}. The $SO(p, p|\mathbb{Z})$ T-duality group is represented by the matrices

$$T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad [30]$$

that act on the matrix

$$E = \frac{r^2}{\alpha'}(G + 2\pi\alpha' B)$$

by a fractional transformation

$$T : E \mapsto E' = (aE + b)(cE + d)^{-1} \quad [31]$$

The transformed metric and B-field are obtained by taking, respectively, the symmetric and antisymmetric parts of E'. The string coupling constant is transformed as

$$T : g_s \mapsto g_s' = \frac{g_s}{(\det(cE + d))^{1/2}} \quad [32]$$

The zero slope limit of Seiberg and Witten is obtained by taking

$$\alpha' \sim \sqrt{\epsilon} \to 0, \qquad G_{ij} \sim \epsilon \to 0 \quad [33]$$

Sending the closed-string metric to zero implies that the B-field dominates in the open-string boundary conditions. In the limit [33], the compactification is parametrized in terms of open-string moduli

$$g_{ij} = -(2\pi\alpha')^2 (BG^{-1}B)_{ij}$$
$$\theta^{ij} = \frac{1}{2\pi r^2}(B^{-1})^{ij} \quad [34]$$

which remain finite. One can demonstrate that θ^{ij} is a noncommutativity parameter for the torus and the low-energy effective theory living on the Dp-brane is a noncommutative maximally supersymmetric gauge theory with a coupling constant

$$G_s = g_s \left(\frac{\det g}{\det G}\right)^{1/4} \quad [35]$$

From the transformation law [31], it is not hard to derive the transformation rules for the moduli [34] in the limit [33],

$$\begin{aligned} T &: g \mapsto g' = (a + b\theta) g (a + b\theta)^t \\ T &: \theta \mapsto \theta' = (c + d\theta)(a + b\theta)^t \end{aligned} \quad [36]$$

Furthermore, the effective gauge theory becomes a noncommutative Yang–Mills theory [17] with a coupling constant

$$(g_{\mathrm{YM}})^{-2} = \frac{(\alpha')^{(3-p)/2}}{(2\pi)^{p-2} G_s}$$

which goes to a finite limit under [33] provided one simultaneously scales g_s with ϵ as

$$g_s \sim \epsilon^{(3-p+k)/4}$$

where k is the rank of B_{ij}. The limiting coupling constant g_{YM} transforms under the T-duality [31], [32] as

$$T : g_{\mathrm{YM}} \mapsto g'_{\mathrm{YM}} = g_{\mathrm{YM}}(\det(a + b\theta))^{1/4} \quad [37]$$

We see that the transformation laws [31] and [37] have the same form as the corresponding transformations in [25], [28], [29] provided one identifies matrix [26] with matrix [30] conjugated by

$$T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The need for conjugation reflects the fact that in the BFSS M(atrix) model in the framework of which the Morita equivalence was originally considered, the natural degrees of freedom are D0 branes versus Dp branes considered in the above discussion of T-duality.

One can further check that the gauge field transformations following from gauge Morita equivalence match with those induced by the T-duality. It is worth stressing that in the absence of a B-field background the effective action based on the square of the gauge field curvature is not invariant under T-duality.

Instantons on Noncommutative T_θ^4

Consider a Yang–Mills field ∇_X on a projective module E over a noncommutative 4-torus T_θ^4. Assume that the Lie algebra of shifts L_θ is equipped with the standard Euclidean metric such that the metric tensor in the basis [7] is given by the identity matrix. The Yang–Mills field ∇_i is called an instanton if the self-dual part of the corresponding curvature tensor is proportional to the identity operator,

$$F_{jk}^+ \equiv \tfrac{1}{2}(F_{jk} + \tfrac{1}{2}\epsilon_{jkmn}F^{mn}) = i\omega_{jk} \cdot \mathbf{1} \quad [38]$$

where ω_{jk} is a constant matrix with real entries. An anti-instanton is defined the same way by replacing the self-dual part with the anti-self-dual one.

One can define a noncommutative analog of Nahm transform for instantons (Astashkevich *et al.* 2000) that has properties very similar to those of the ordinary (commutative) one. To that end, consider a triple $(\mathcal{P}, \nabla_i, \hat{\nabla}_i)$ consisting of a (finite projective) $(T_\theta^4, T_{\hat{\theta}}^4)$-bimodule $\mathcal{P}$, T_θ^4-connection ∇_i and $T_{\hat{\theta}}^4$-connection $\hat{\nabla}_i$ that satisfy the following properties. The connection ∇_i commutes with the $T_{\hat{\theta}}$-action on $\mathcal{P}$ and the connection $\hat{\nabla}_i$ with that of T_θ. The commutators $[\nabla_i, \nabla_j], [\hat{\nabla}_i, \hat{\nabla}_j], [\nabla_i, \hat{\nabla}_j]$ are proportional to the identity operator

$$[\nabla_i, \nabla_j] = \omega_{ij} \cdot \mathbf{1}$$
$$[\hat{\nabla}_i, \hat{\nabla}_j] = \hat{\omega}_{ij} \cdot \mathbf{1} \quad [39]$$
$$[\nabla_i, \hat{\nabla}_j] = \sigma_{ij} \cdot \mathbf{1}$$

The above conditions mean that $\mathcal{P}$ is a $T^8_{\theta \oplus (-\hat{\theta})}$-module and $\nabla_i \oplus \hat{\nabla}_i$ is a constant curvature connection on it. In addition, we assume that the tensor σ_{ij} is nondegenerate.

For a connection ∇^E on a right T^4_θ-module E, we define a Dirac operator $D = \Gamma^i(\nabla^E_i + \nabla_i)$ acting on the tensor product

$$(E \otimes_{T_\theta} \mathcal{P}) \otimes S$$

where S is the SO(4) spinor representation space and Γ^i are four-dimensional Dirac gamma-matrices. The space S is $\mathbb{Z}_2$-graded: $S = S^+ \oplus S^-$ and D is an odd operator so that we can consider

$$D^+ : (E \otimes_{T_\theta} \mathcal{P}) \otimes S^+ \to (E \otimes_{T_\theta} \mathcal{P}) \otimes S^-$$
$$D^- : (E \otimes_{T_\theta} \mathcal{P}) \otimes S^- \to (E \otimes_{T_\theta} \mathcal{P}) \otimes S^+$$

A connection ∇^E_i on a T^4_θ-module E is called $\mathcal{P}$-irreducible if there exists a bounded inverse to the Laplacian

$$\Delta = \sum_i (\nabla^E_{\mathrm{i}} + \nabla_i)(\nabla^E_{\mathrm{i}} + \nabla_i)$$

One can show that if ∇^E is a $\mathcal{P}$-irreducible instanton, then $\ker D^+ = 0$ and $D^- D^+ = \Delta$. Denote by $\hat{E}$ the closure of the kernel of D^-. Since D^- commutes with the $T^4_{\hat{\theta}}$-action on $(E \otimes_{T_\theta} \mathcal{P}) \otimes S^-$ the space $\hat{E}$ is a right $T^4_{\hat{\theta}}$-module. One can prove that this module is finite projective. Let $P : (E \otimes_{T_\theta} \mathcal{P}) \otimes S^- \to \hat{E}$ be a Hermitian projector. Denote by $\nabla^{\hat{E}}$ the composition $P \circ \hat{\nabla}$. One can show that $\nabla^{\hat{E}}$ is a Yang–Mills field on $\hat{E}$.

The noncommutative Nahm transform of a $\mathcal{P}$-irreducible instanton connection ∇^E on E is defined to be the pair $(\hat{E}, \nabla^{\hat{E}})$. One can further show that $\nabla^{\hat{E}}$ is an instanton.

See also: Electroweak Theory; Hopf Algebras and q-Deformation Quantum Groups; Noncommutative Geometry from Strings; Quantum Group Differentials, Bundles and Gauge Theory; Quantum Hall Effect; String Field Theory; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory.

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Nonequilibrium Statistical Mechanics (Stationary): Overview

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Nonequilibrium

Systems in stationary nonequilibrium are mechanical systems subject to nonconservative external forces and to thermostat forces which forbid indefinite increase of the energy and allow reaching statistically stationary states. A system Σ is described by the positions and velocities of its n particles $X, \dot{X}$, with the particle positions confined to a finite volume container C_0.

If $X = (x_1, \ldots, x_n)$ are the particle positions in a Cartesian inertial system of coordinates, the equations of motion are determined by their masses $m_i > 0$, $i = 1, \ldots, n$, by the potential energy of

interaction $V(x_1,\dots,x_n) \equiv V(X)$, by the external nonconservative forces $F_i(X,\Phi)$, and by the thermostat forces $-\vartheta_i$ as

$$m_i\ddot{x}_i = -\partial_{x_i}V(X) + F_i(X;\Phi) - \vartheta_i, \quad i=1,\dots,n \qquad [1]$$

where $\Phi=(\varphi_1,\dots,\varphi_q)$ are strength parameters on which the external forces depend. All forces and potentials will be supposed smooth, that is, analytic, in their variables aside from possible impulsive elastic forces describing shocks, and with the property $F(X;0)=0$. The impulsive forces are allowed here to model possible shocks with the walls of the container C_0 or between hard core particles.

A thermostat is a "reservoir" which may consist of one or more infinite systems which are asymptotically in thermal equilibrium and are separated by boundary surfaces from each other as well as from the system: with the latter, they interact through short-range conservative forces, see **Figure 1**.

The reservoirs occupy infinite regions of the space outside C_0, for example, sectors $C_a \subset \mathbb{R}^3, a=1,2\dots$, in space and their particles are in a configuration which is typical of an equilibrium state at temperature T_a. This means that the empirical probability of configurations in each C_a is Gibbsian with some temperature T_a. In other words, the frequency with which a configuration $(\dot{Y}, Y+r)$ occurs in a region $\Lambda + r \subset C_a$ while a configuration $(\dot{W}, W+r)$ occurs outside $\Lambda + r$ (with $Y \subset \Lambda, W \cap \Lambda = \emptyset$) averaged over the translations $\Lambda + r$ of Λ by r (with the restriction that $\Lambda + r \subset C_a$) is

$$\underset{r+\Lambda\subset C_a}{\text{average}}(f_{\Lambda+r}[(\dot{Y}, Y+r); \dot{W}, W+r]) = \frac{e^{-\beta_a\left((1/2m_a)|\dot{Y}|^2 + V_a(Y|W)\right)}}{\text{normalization}} \qquad [2]$$

Here m_a is the mass of the particles in the ath reservoir and $V_a(Y|W)$ is the energy of the short-range potential between pairs of particles in $Y \subset C_a$ or with one point in Y and one in W. Since the configurations in the system and in the thermostats are not random, [2] should be considered as an "empirical" probability in the sense that it is the frequency density of the events $\{(\dot{Y}, Y+r); W+r\}$: in other words, the configurations ω_a in the reservoirs should be "typical" in the sense of probability theory of distributions which are asymptotically Gibbsian.

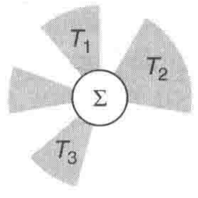


Figure 1 A symbolic drawing of the container C_0 for the system Σ and of the surrounding regions containing the particles acting as thermostats at temperatures $T_1, T_2, \dots$.

The property of being "thermostats" means that [2] remains true for all times, if initially satisfied.

Mathematically, there is a problem at this point: the latter property is either true or false, but a proof of its validity seems out of reach of the present techniques except in very simple cases. Therefore, here we follow an intuitive approach and assume that such thermostats exist and, actually, that any configuration which is typical of a stationary state of an infinite size system of interacting particles in the C_a's, with physically reasonable microscopic interactions, satisfies the property [2].

The above thermostats are examples of "deterministic thermostats" because, together with the system, they form a deterministic dynamical system. They are called "Hamiltonian thermostats" and are often considered as the most appropriate models of "physical thermostats."

A closely related thermostat model is obtained by assuming that the particles outside the system are not in a given configuration but they have a probability distribution whose conditional distributions satisfy [2] initially. Also in this case, it is necessary to assume that [2] remains true for all times, if initially satisfied. Such thermostats are examples of "stochastic thermostats" because their action on the system depends on random variables ω_a which are the initial configurations of the particles belonging to the thermostats.

Other kinds of stochastic thermostats are "collision rules" with the container boundary ∂C_0 of Σ: every time a particle collides with ∂C_0 it is reflected with a momentum p in d^3p that has a probability distribution proportional to $e^{-\beta_a(1/2m)p^2}d^3p$ where $\beta_a, a=1,2,\dots$ depends on which boundary portion (labeled by $a=1,2,\dots$) the collision takes place and $T_a=(k_B\beta_a)^{-1}$ and its "temperature" if k_B is Boltzmann's constant. Which p is actually chosen after each collision is determined by a random variable $\omega=(\omega_1,\omega_2,\dots)$.

The distinction between stochastic and deterministic thermostats ultimately rests on what we call "system." If reservoirs or the randomness generators are included in the system, then the system becomes deterministic (possibly infinite); and finite deterministic thermostats can also be regarded as simplified models for infinite reservoirs, see the section "Heat, temperature, and entropy production."

It is also possible, and convenient, to consider "finite deterministic thermostats." In the latter case, $\boldsymbol{\vartheta}$ is a force only depending upon the configuration of the n particles v of Σ in their finite container C_0.

Examples of finite deterministic reservoirs are forces obtained by imposing a nonholonomic constraint via some *ad hoc* principle like the *Gauss principle.* For instance, if a system of particles driven by a force $\boldsymbol{G}_i \stackrel{\text{def}}{=} -\partial_{\boldsymbol{x}_i} V(\boldsymbol{X}) + \boldsymbol{F}_i(\boldsymbol{X})$ is enclosed in a box C_0 and $\boldsymbol{\vartheta}$ is a thermostat enforcing an anholonomic constraint $\psi(\dot{\boldsymbol{X}}, \boldsymbol{X}) \equiv 0$ via Gauss' principle, then

$$\boldsymbol{\vartheta}_i(\dot{\boldsymbol{X}}, \boldsymbol{X}) = \left[\frac{\sum_j \dot{\boldsymbol{x}}_j \cdot \partial_{\boldsymbol{x}_j}\psi(\dot{\boldsymbol{X}}, \boldsymbol{X}) + (1/m)\boldsymbol{G}_j \cdot \partial_{\dot{\boldsymbol{x}}_j}\psi(\dot{\boldsymbol{X}}, \boldsymbol{X})}{\sum_j \frac{1}{m}(\partial_{\dot{\boldsymbol{x}}_j}\psi(\dot{\boldsymbol{X}}, \boldsymbol{X}))^2}\right] \times \partial_{\dot{\boldsymbol{x}}_i}\psi(\dot{\boldsymbol{X}}, \boldsymbol{X}) \qquad [3]$$

Gauss' principle says that the force which needs to be added to the other forces $\boldsymbol{G}_i$ acting on the system minimizes

$$\sum_i \frac{(\boldsymbol{G}_i - m_i \boldsymbol{a}_i)^2}{m_i}$$

given $\dot{\boldsymbol{X}}, \boldsymbol{X}$, among all accelerations $\boldsymbol{a}_i$ which are compatible with the constraint ψ.

It should be kept in mind that the only known examples of mathematically treatable thermostats modeled by infinite reservoirs are cases in which the thermostat particles are either noninteracting particles or linear (i.e., noninteracting) oscillators. For simplicity stochastic or infinite thermostats will not be considered here and we restrict attention to finite deterministic systems.

In general, in order that a force $\boldsymbol{\vartheta}$ can be considered a deterministic "thermostat force" a further property is necessary: namely that the system evolves according to [1] towards a stationary state. This means that for all initial particle configurations $(\dot{\boldsymbol{X}}, \boldsymbol{X})$, except possibly for a set of zero phase-space volume, any smooth function $f(\dot{\boldsymbol{X}}, \boldsymbol{X})$ evolves in time so that, if $S_t(\dot{\boldsymbol{X}}, \boldsymbol{X})$ denotes the configuration into which the initial data evolve in time t according to [1], then the limit

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T f(S_t(\dot{\boldsymbol{X}}, \boldsymbol{X}))\,\mathrm{d}t = \int f(z)\mu(\mathrm{d}z) \qquad [4]$$

exists and is independent of $(\dot{\boldsymbol{X}}, \boldsymbol{X})$. The probability distribution μ is then called the SRB distribution for the system. The maps S_t will have the group property $S_t \cdot S_{t'} = S_{t+t'}$ and the SRB distribution μ will be invariant under time evolution.

It is important to stress that the requirement that the exceptional configurations form just a set of zero phase volume (rather than a set of zero probability with respect to another distribution, singular with respect to the phase volume) is a strong assumption and it should be considered an axiom of the theory: it corresponds to the assumption that the initial configuration is prepared as a typical configuration of an equilibrium state, which, by the classical equidistribution axiom of equilibrium statistical mechanics, is a typical configuration with respect to the phase volume.

For this reason, the SRB distribution is said to describe a "stationary nonequilibrium state" of the system. The SRB distribution depends on the parameters on which the forces acting on the system depend, for example, $|C_0|$ (volume), $\boldsymbol{\Phi}$ (strength of the forcings), $\{\beta_a^{-1}\}$ (temperatures), etc. The collection of SRB distributions obtained by letting the parameters vary defines a "nonequilibrium ensemble."

In the stochastic case, the distribution μ is required to be invariant in the sense that it can be regarded as a marginal distribution of an invariant distribution for the larger (deterministic) system formed by the thermostats and the system itself.

For more details, the reader is referred to Evans and Morriss (1990), Ruelle (1999), and Eckmann *et al.* (1999).

Nonequilibrium Thermodynamics

The key problem of nonequilibrium statistical mechanics is to derive a macroscopic "nonequilibrium thermodynamics" in a way similar to the derivation of equilibrium thermodynamics from equilibrium statistical mechanics.

The first difficulty is that nonequilibrium thermodynamics is not well understood. For instance, there is no (agreed upon) definition of entropy of a nonequilibrium stationary state, while it should be kept in mind that the effort to find the microscopic interpretation of equilibrium entropy, as defined by Clausius, was a driving factor in the foundations of equilibrium statistical mechanics.

The importance of entropy in classical equilibrium thermodynamics rests on the implication of universal, parameter-free relations which follow from its existence (e.g., $\partial_V(1/T) \equiv \partial_U(p/T)$ if U is the internal energy, T the absolute temperature, and p the pressure of a simple homogeneous material).

Are there universal relations among averages of observables with respect to SRB distributions?

The question has to be posed for systems "really" out of equilibrium, that is, for $\boldsymbol{\Phi} \neq 0$ (see [1]): in fact, there is a well-developed theory of the derivatives with respect to $\boldsymbol{\Phi}$ of averages of

observables evaluated at $\Phi = 0$. The latter theory is often called, and here we shall do so as well, "classical nonequilibrium thermodynamics" or "near-equilibrium thermodynamics" and it has been quite successfully developed on the basis of the notions of equilibrium thermodynamics, paying particular attention to the macroscopic evolution of systems described by macroscopic continuum equations of motion.

"Stationary nonequilibrium statistical mechanics" will indicate a theory of the relations between averages of observables with respect to SRB distributions. Systems so large that their volume elements can be regarded as being in locally stationary nonequilibrium states could also be considered. This would extend the familiar "local equilibrium states" of classical nonequilibrium thermodynamics: however, they are not considered here. This means that we shall not attempt to find the macroscopic equations regulating the time evolution of continua locally in nonequilibrium stationary states but we shall only try to determine the properties of their "volume elements" assuming that the timescale for the evolution of large assemblies of volume elements is slow compared to the timescales necessary to reach local stationarity.

For more details, the reader is referred to de Groot and Mazur (1984), Lebowitz (1993), Ruelle (1999, 2000), Gallavotti (1998, 2004), and Goldstein and Lebowitz (2004).

Chaotic Hypothesis

In equilibrium statistical mechanics, the ergodic hypothesis plays an important conceptual role as it implies that the motions of ergodic systems have an SRB statistics and that the latter coincides with the Liouville distribution on the energy surface.

An analogous role has been proposed for the "chaotic hypothesis," which states that the

motion of a chaotic system, developing on its attracting set, can be regarded as an Anosov flow.

This means that the attracting sets of chaotic systems, physically defined as systems with at least one positive Lyapunov exponent, can be regarded as smooth surfaces on which motion is highly unstable:

1. Around every point, a curvilinear coordinate system can be established which has three planes, varying continuously with x, which are covariant (i.e., they are coordinate planes at a point x which are mapped, by the evolution S_t, into the corresponding coordinate planes around $S_t x$).
2. The planes are of three types, "stable," "unstable," and "marginal," with respective positive dimensions d_s, d_u, and 1: infinitesimal lengths on the stable plane and on the unstable plane of any point contract at exponential rate as time proceeds towards the future or towards the past. The length along the marginal direction neither contracts nor expands (i.e., it varies around the initial value staying bounded away from 0 and ∞): its tangent vector is parallel to the flow. In cases in which time evolution is discrete, and determined by a map S, the marginal direction is missing.
3. The contraction over a time t, positive for lines on the stable plane and negative for those on the unstable plane, is exponential, i.e. lengths are contracted by a factor uniformly bounded by $Ce^{-\kappa|t|}$ with $C, \kappa > 0$.
4. There is a dense trajectory.

It has to be stressed that the chaotic hypothesis concerns physical systems: mathematically, it is very easy to find dynamical systems for which it does not hold, at least as easy as it is to find systems in which the ergodic hypothesis does not hold (e.g., harmonic lattices or blackbody radiation). However, if suitably interpreted, the ergodic hypothesis leads, even for these systems, to physically correct results (the specific heats at high temperature, the Raleigh–Jeans distribution at low frequencies). Moreover, the failures of the ergodic hypothesis in physically important systems have led to new scientific paradigms (like quantum mechanics from the specific heats at low temperature and Planck's law).

Since physical systems are almost always not Anosov systems, it is very likely that probing motions in extreme regimes will make visible the features that distinguish Anosov systems from non-Anosov systems, much as it happens with the ergodic hypothesis.

The interest of the hypothesis is to provide a framework in which properties like the existence of an SRB distribution is *a priori* guaranteed, together with an expression for it which can be used to work with formal expressions of the averages of the observables: the role of Anosov systems in chaotic dynamics is similar to the role of harmonic oscillators in the theory of regular motions. They are the paradigm of chaotic systems, as the harmonic oscillators are the paradigm of order. Of course, the hypothesis is only a beginning and one has to learn how to extract information from it, as it was the case with the use of the Liouville distribution, once the ergodic hypothesis guaranteed that it was the

appropriate distribution for the study of the statistics of motions in equilibrium situations.

For more details, the reader is referred to Ruelle (1976), Gallavotti and Cohen (1995), Ruelle (1999), Gallavotti (1998), and Gallavotti *et al.* (2004).

Heat, Temperature, and Entropy Production

The amount of *heat* $\dot{Q}$ that a system produces while in a stationary state is naturally identified with the work that the thermostat forces $\boldsymbol{\vartheta}$ perform per unit time

$$\dot{Q} = \sum_i \boldsymbol{\vartheta}_i \cdot \dot{\boldsymbol{x}}_i \qquad [5]$$

A system may be in contact with several reservoirs: in models, this will be reflected by a decomposition

$$\boldsymbol{\vartheta} = \sum \boldsymbol{\vartheta}^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X}) \qquad [6]$$

where $\boldsymbol{\vartheta}^{(a)}$ is the force due to the ath thermostat and depends on the coordinates of the particles which are in a region $\Lambda_a \subseteq C_0$ of a decomposition $\cup_{a=1}^m \Lambda_a = C_0$ of the container C_0 occupied by the system ($\Lambda_a \cap \Lambda_{a'} = \emptyset$ if $a \neq a'$).

From several studies based on simulations of finite thermostatted systems of particles arose the proposal to consider the average of the phase-space contraction $\sigma^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X})$ due to the ath thermostat

$$\sigma^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X}) \stackrel{\text{def}}{=} \sum_j \partial_{\dot{x}_j} \cdot \boldsymbol{\vartheta}_j^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X}) \qquad [7]$$

and to identify it with the *rate of entropy creation* in the ath thermostat.

Another key notion in thermodynamics is the temperature of a reservoir; in the infinite deterministic thermostat case, of the section "Nonequilibrium," it is defined as $(k_{\rm B}\beta_a)^{-1}$ but in the finite deterministic thermostats considered here it needs to be defined. If there are m reservoirs with which the system is in contact, one sets

$$\begin{aligned} \sigma_+^{(a)} &\stackrel{\text{def}}{=} \langle \sigma^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X}) \rangle \equiv \int \sigma^{(a)}(\dot{\boldsymbol{X}}, \boldsymbol{X})\, \mu(\mathrm{d}\dot{\boldsymbol{X}}\, \mathrm{d}\boldsymbol{X}) \\ \dot{Q}_a &\stackrel{\text{def}}{=} \sum_i \boldsymbol{\vartheta}_i^{(a)} \cdot \dot{\boldsymbol{x}}_i \end{aligned} \qquad [8]$$

where μ is the SRB distribution describing the stationary state. It is natural to define the absolute temperature of the ath thermostat to be

$$T_a = \frac{\langle \dot{Q}_a \rangle}{k_{\rm B} \sigma_+^{(a)}} \qquad [9]$$

It is not clear that $T_a > 0$: this happens in a rather general class of models and it would be desirable, for the interpretation that is proposed here, that it could be considered a property to be added to the requirements that the forces $\boldsymbol{\vartheta}^{(a)}$ be thermostat models.

An important class of thermostats for which the property $T_a > 0$ holds can be described as follows. Imagine N particles in a container C_0 interacting via a potential $V_0 = \sum_{i<j} \varphi(q_i - q_j) + \sum_j V'(q_j)$ (where V' models external conservative forces like obstacles, walls, gravity, ...) and, furthermore, interacting with M other systems Σ_a, of N_a particles of mass m_a, in containers C_a contiguous to C_0. The latter will model M parts of the system in contact with thermostats at temperatures $T_a, a = 1, \ldots, M$.

The coordinates of the particles in the ath system Σ_a will be denoted $\boldsymbol{x}_j^a, j = 1, \ldots, N_a$, and they will interact with each other via a potential $V_a = \sum_{i,j}^{N_a} \varphi_a(\boldsymbol{x}_i^a - \boldsymbol{x}_j^a)$. Furthermore, there will be an interaction between the particles of each thermostat and those of the system via potentials $W_a = \sum_{i=1}^N \sum_{j=1}^{N_a} w_a(q_i - \boldsymbol{x}_j^a), a = 1, \ldots, M$.

The potentials will be assumed to be either hard core or nonsingular potentials and the external V' is supposed to be at least such that it forbids the existence of obvious constants of motion.

The temperature of each Σ_a will be defined by the total kinetic energy of its particles, that is, by $K_a = \sum_{j=1}^{N_a} (1/2) m_a (\dot{\boldsymbol{x}}_j^a)^2 \stackrel{\text{def}}{=} (3/2) N_a k_{\rm B} T_a$: the particles of the ath thermostat will be kept at constant temperature by further forces $\boldsymbol{\vartheta}_j^a$. The latter are defined by imposing via a Gaussian constraint that K_a is a constant of motion (see [3] with $\psi \equiv K_a$). This means that the equations of motion are

$$\begin{aligned} m\ddot{\boldsymbol{q}}_j &= -\partial_{q_j}\left(V_0(\boldsymbol{Q}) + \sum_{a=1}^{N_a} W_a(\boldsymbol{Q}, \boldsymbol{x}^a) \right) \\ m_a \ddot{\boldsymbol{x}}_j^a &= -\partial_{\boldsymbol{x}_j^a}(V_a(\boldsymbol{x}^a) + W_a(\boldsymbol{Q}, \boldsymbol{x}^a)) - \boldsymbol{\vartheta}_j^a \end{aligned} \qquad [10]$$

and an application of Gauss' principle yields

$$\boldsymbol{\vartheta}_j^a = \frac{L_a - \dot{V}_a}{3 N_a k_{\rm B} T_a} \dot{\boldsymbol{x}}_j^a \stackrel{\text{def}}{=} \alpha^a \dot{\boldsymbol{x}}_j^a$$

where L_a is the work per unit time done by the particles in C_0 on the particles of Σ_a and V_a is their potential energy.

In this case, the partial divergence $\sigma^a \equiv (3N_a - 1)\alpha^a$ is, up to a constant factor $(1 - (1/3N_a))$,

$$\sigma^a = \frac{L_a}{k_{\rm B} T_a} - \frac{\dot{V}_a}{k_{\rm B} T_a}$$

and it will make [9] identically satisfied with $T_a > 0$ because L_a can be naturally interpreted as heat Q_a ceded, per unit time, by the particles in C_0 to the subsystem Σ_a (hence to the ath thermostat because the temperature of Σ_a is constant), while the

derivative of V_a will not contribute to the value of σ_+^a. The phase-space contraction rate is, neglecting the total derivative terms (and $O(N_a^{-1})$),

$$\sigma_{\text{true}}(\dot{X},X)=\sum_{a=1}^{N_a}\frac{\dot{Q}_a}{k_B T_a} \qquad [11]$$

where the subscript "true" is to remind that an additive total derivative term distinguishes it from the complete phase-space contraction.

Remarks

(i) The above formula provides the motivation of the name "entropy creation rate" attributed to the phase-space contraction σ. Note that in this way the definition of entropy creation is "reduced" to the equilibrium notion because what is being defined is the entropy increase of the thermostats which have to be considered in equilibrium. No attempt is made here to define neither the entropy of the stationary state nor the notion of temperature of the nonequilibrium system in C_0 (the T_a are temperatures of the Σ_a, not of the particles in C_0). This is an important point as it leaves open the possibility of envisaging the notion of "local equilibrium" which becomes necessary in the approximation (not considered here) in which the system is regarded as a continuum.

(ii) In the above model, another viewpoint is possible: that is, to consider the system to consist of only the N particles in C_0 and the M systems Σ_a to be thermostats. From this point of view, it can be considered a model of a system subject to thermostats. The Gibbs distribution characterizing the infinite thermostats of the section "Nonequilibrium" becomes in this case the constraint that the kinetic energies K_a are constants, enforced by the Gaussian forces. In the new viewpoint, the appropriate definition should be simply the right-hand side (RHS) of [11], i.e. the work per unit time done by the forces of the system on the thermostats divided by the temperature of the thermostats. This suggests a different and general definition of entropy creation rate, applying also to thermostats that are often considered "more physical" and that needs to be further investigated. In the example [10] the new definition differs from the phase space contraction rate by a total time derivative, i.e. rather trivially for the purposes of the following.

For more details, the reader is referred to Evans and Morriss (1990), Gallavotti and Cohen (1995), Ruelle (1996, 1997), and Gallavotti (2004).

Thermodynamic Fluxes and Forces

Nonequilibrium stationary states depend upon external parameters φ_j like the temperatures T_a of the thermostats or the size of the force parameters $\mathbf{\Phi}=(\varphi_1,\ldots,\varphi_q)$, see [1]. Nonequilibrium thermodynamics is well developed at "low forcing": strictly speaking, this means that it is widely believed that we understand the properties of the derivatives of the averages of observables with respect to the external parameters if evaluated at $\varphi_j=0$. Important notions are the notions of thermodynamic fluxes J_i and of thermodynamic forces φ_i; hence, it seems important to extend such notions to nonequilibrium systems (i.e., $\mathbf{\Phi}\neq 0$).

A possible extension could be to define the thermodynamic flux J_i associated with a force φ_i as $J_i=\langle\partial_{\varphi_i}\sigma\rangle_{\text{SRB}}$ where $\sigma(X,\dot{X};\mathbf{\Phi})$ is the volume contraction per unit time. This definition seems appropriate in several concrete cases that have been studied and it is appealing for its generality.

An interesting example is provided by the model of thermostatted system in [10]: if the container of the system is a box with periodic boundary conditions, one can imagine to add an extra constant force E acting on the particles in the container. Imagining the particles to be charged by a charge e and regarding such force as an electric field, the first equation in [10] is modified by the addition of a term eE.

The constraints on the thermostat temperatures imply that σ depends also on E: in fact, if $\boldsymbol{J}=e\sum_j\dot{q}_j$ is the electric current, energy balance implies $\dot{U}_{\text{tot}}=\boldsymbol{E}\cdot\boldsymbol{J}-\sum_a(L_a-\dot{V}_a)$ if U_{tot} is the sum of all kinetic and potential energies. Then, the phase-space contraction

$$\sum_a\frac{L_a-\dot{V}_a}{T_a}$$

can be written, to first order in the temperature variations δT_a with respect to a common value $T_a=T$, as

$$-\sum_a\frac{L_a-\dot{V}_a}{T}\frac{\delta T_a}{T}+\frac{\boldsymbol{E}\cdot\boldsymbol{J}-\dot{U}_{\text{tot}}}{T}$$

hence σ_{true}, see [11], is

$$\sigma_{\text{true}}=\frac{\boldsymbol{E}\cdot\boldsymbol{J}}{k_B T}-\sum_a\frac{\dot{Q}_a}{k_B T}\frac{\delta T_a}{T} \qquad [12]$$

The definition and extension of the conjugacy between thermodynamic forces and fluxes is compatible with the key results of classical nonequilibrium thermodynamics, at least as far as Onsager

reciprocity and Green–Kubo's formulas are concerned. It can be checked that if the equilibrium system is reversible, that is, if there is an isometry I on phase space which anticommutes with the evolution ($IS_t = S_{-t}I$ in the case of continuous-time dynamics $t \to S_t$ or $IS = S^{-1}I$ in the case of discrete-time dynamics S), then, shortening $(\dot{X}, X)$ into x,

$$L_{ij} \stackrel{\text{def}}{=} \partial_{\Phi_i} J_j|_{\Phi=0} = \partial_{\Phi_i} \langle \partial_{\Phi_j} \sigma(x;\Phi) \rangle_{\text{SRB}}|_{\Phi=0} = \partial_{\Phi_j} J_i|_{\Phi=0}$$
$$= L_{ji} = \frac{1}{2} \int_{-\infty}^{\infty} \langle \partial_{\Phi_i} \sigma(S_t x;\Phi) \partial_{\Phi_j} \sigma(x;\Phi) \rangle_{\text{SRB}}|_{\Phi=0}\, \text{d}t \qquad [13]$$

The $\sigma(x;\Phi)$ plays the role of "Lagrangian" generating the duality between forces and fluxes. The extension of the duality just considered might be of interest in situations in which $\Phi \neq 0$.

For more details, the reader is referred to de Groot and Mazur (1984), Gallavotti (1996), and Gallavotti and Ruelle (1997).

Fluctuations

As in equilibrium, large statistical fluctuations of observables are of great interest and already there is, at the moment, a rather large set of experiments dedicated to the analysis of large fluctuations in stationary states out of equilibrium.

If one defines the dimensionless phase-space contraction

$$p(x) = \frac{1}{\tau} \int_0^{\tau} \frac{\sigma(S_t x)}{\sigma_+}\, \text{d}t \qquad [14]$$

(see also [11]), then there exists $p^* \geq 1$ such that the probability P_τ of the event $p \in [a,b]$ with $[a,b] \subset (-p^*, p^*)$ has the form

$$P_\tau(p \in [a,b]) = \text{const. } e^{\tau \max_{p \in [a,b]} \zeta(p) + O(1)} \qquad [15]$$

with $\zeta(p)$ analytic in $(-p^*, p^*)$. The function $\zeta(p)$ can be conveniently normalized to have value 0 at $p = 1$ (i.e., at the average value of p).

Then, in Anosov systems which are reversible and dissipative (see the previous section), a general symmetry property, called the "fluctuation theorem" and reflecting the reversibility symmetry, yields the parameterless relation

$$\zeta(-p) = \zeta(p) - p\sigma_+ \quad p \in (-p^*, p^*) \qquad [16]$$

This relation is interesting because it has no free parameters; in other words, it is universal for reversible dissipative Anosov systems. In connection with the flux–force duality in the previous section, it can be checked to reduce to the Green–Kubo formula and to Onsager reciprocity, see [13], in the case in which the evolution depends on several fields Φ and $\Phi \to 0$ (of course the relation becomes trivial as $\Phi \to 0$ because $\sigma_+ \to 0$ and to obtain the result one has first to divide both sides by suitable powers of the fields Φ).

A more informal (but imprecise) way of writing [15] and [16] is

$$\frac{P_\tau(p)}{P_\tau(-p)} = e^{\tau p \sigma_+ + O(1)}, \quad \text{for all } p \in (-p^*, p^*) \qquad [17]$$

where $P_\tau(p)$ is the probability density of p. An obvious but interesting consequence of [17] is that

$$\langle e^{-\tau p \sigma_+} \rangle_{\text{SRB}} = 1$$

in the sense that $(1/\tau) \log \langle e^{-\tau p \sigma_+} \rangle_{\text{SRB}} \xrightarrow[\tau \to \infty]{} 0$.

Occasionally, systems with singularities have to be considered. In such cases, the relation [16] may change in the sense that the function $\zeta(p)$ may not be analytic: in such cases, one expects that the relation holds in the largest analyticity interval symmetric around the origin. In Anasov systems and also various cases considered in the literature, such interval appears to contain the interval $(-1, 1)$.

Note that in the theory of fluctuations of the time averages p we can replace σ by any other *bounded* quantity which is a total time derivative: hence, in the example discussed above, it can be replaced by σ_{true}, see [12], which has a natural physical meaning.

It is important to remark that the above fluctuation relation is the first representative of several consequences of the reversibility and chaotic hypotheses. For instance, given $F_1, \ldots, F_n$ arbitrary observables which are (say) odd under time reversal I (i.e., $F(Ix) = -F(x)$) and given n functions $t \in [-\tau/2, \tau/2] \to \varphi_j(t), j = 1, \ldots, n$, one can ask which is the probability that $F_j(S_t x)$ "closely follows" the "pattern" $\varphi_j(t)$ and at the same time

$$\frac{1}{\tau} \int_0^{\tau} \frac{\sigma(S_\theta x)}{\sigma_+}\, \text{d}\theta$$

has value p. Then calling $P_\tau(F_1 \sim \varphi_1, \ldots, F_n \sim \varphi_n, p)$ the probability of this event, which we write in the imprecise form corresponding to [17] for simplicity, and defining $I\varphi_j(t) \stackrel{\text{def}}{=} -\varphi_j(-t)$, it is

$$\frac{P_\tau(F_1 \sim \varphi_1, \ldots, F_n \sim \varphi_n, p)}{P_\tau(F_1 \sim I\varphi_1, \ldots, F_n \sim I\varphi_n, -p)} = e^{\tau\sigma_+ p}$$
$$p \in (-p^*, p^*) \qquad [18]$$

which is remarkable because it is parameterless and at the same time surprisingly independent of the choice of the observables F_j. The relation [18] has far-reaching consequences: for instance, if $n = 1$ and $F_1 = \partial_{\Phi_i} \sigma(x;\Phi)$ the relation [18] has been used to derive the mentioned Onsager reciprocity and Green–Kubo's formulas at $\Phi = 0$.

Equation [18] can be read as follows: the probability that the observables F_j follow given evolution patterns φ_j conditioned to entropy creation rate $p\sigma_+$ is the same that they follow the time-reversed patterns if conditioned to entropy creation rate $-p\sigma_+$. In other words, to change the sign of time, it is just sufficient to reverse the sign of entropy creation rate, no "extra effort" is needed.

For more details, the reader is referred to Sinai (1972, 1994), Evans *et al.* (1993), Gallavotti and Cohen (1995), Gallavotti (1996, 1999), Gallavotti and Ruelle (1997), Gallavotti *et al.* (2004), and Bonetto *et al.* (2005).

Fractal Attractors, Pairing, and Time Reversal

Attracting sets (i.e., sets which are the closure of attractors) are fractal in most dissipative systems. However, the chaotic hypothesis assumes that fractality can be neglected. Apart from the very interesting cases of systems close to equilibrium, in which the closure of an attractor is the whole phase space (under the chaotic hypothesis, i.e., if the system is Anosov), hence not fractal, serious problems arise in preserving validity of the fluctuation theorem.

The reason is very simple: if the attractor closure is smaller than phase space, then it is to be expected that time reversal will change the attractor into a repeller disjoint from it. Thus, even if the chaotic hypothesis is assumed, so that the attracting set $\mathcal{A}$ can be considered a smooth surface, the motion on the attractor will not be time-reversal symmetric (as its time-reversal image will develop on the repeller). One can say that an attracting set with dimension lower than that of phase space in a time-reversible system corresponds to a spontaneous breakdown of time-reversal symmetry.

It has been noted however that there are classes of systems, forming a large set in the space of evolutions depending on a parameter Φ, in which geometric reasons imply that if beyond a critical value Φ_c the attracting set becomes smaller than phase space, then a map I_P is generated mapping the attractor $\mathcal{A}$ into the repeller $\mathcal{R}$, and vice versa, such that I_P^2 is the identity on $\mathcal{A}\cup\mathcal{R}$ and I_P commutes with the evolution: therefore, the composition $I\cdot I_P$ is a time-reversal symmetry (i.e., it anticommutes with evolution) for the motions on the attracting set $\mathcal{A}$ (as well as on the repeller $\mathcal{R}$).

In other words, the time-reversal symmetry in such systems "cannot be broken": if spontaneous breakdown occurs (i.e., $\mathcal{A}$ is not mapped into itself under time reversal I), a new symmetry I_P is spawned and $I\cdot I_P$ is a new time-reversal symmetry (an analogy with the spontaneous violation of time reversal in quantum theory, where time reversal T is violated but TCP is still a symmetry: so T plays the role of I and CP that of I_P).

Thus, a fluctuation relation will hold for the phase-space contraction of the motions taking place on the attracting set for the class of systems with the geometric property mentioned above (technically, the latter is called "axiom C" property).

This is interesting but it still is quite far from being checkable even in numerical experiments. There are nevertheless systems in which a "pairing property" also holds: this means that, considering the case of discrete-time maps S, the Jacobian matrix $\partial_x S(x)$ has $2N$ eigenvalues that can be labeled, in decreasing order, $\lambda_N(x),\ldots,\lambda_{(1/2)N}(x),\ldots,\lambda_1(x)$, with the remarkable property that $(1/2)(\lambda_{N-j}(x)+\lambda_j(x))\stackrel{\text{def}}{=}\alpha(x)$ is j-independent. In such systems, a relation can be established between phase-space contractions in the full phase space and on the surface of the attracting set: the fluctuation theorem for the motion on the attracting set can therefore be related to the properties of the fluctuations of the total phase-space contraction measured on the attracting set (which includes the contraction transversal to the attracting set) and if $2M$ is the attracting set dimension and $2N$ is the total dimension of phase space it is, in the analyticity interval $(-p^*,p^*)$ of the function $\zeta(p)$,

$$\zeta(-p)=\zeta(p)-p\frac{M}{N}\sigma_+ \qquad [19]$$

which is an interesting relation. It is however very difficult to test in mechanical systems because in such systems it seems very difficult to make the field so high to see an attracting set thinner than the whole phase space and still observe large fluctuations.

For more details, the reader is referred to Dettman and Morriss (1996) and Gallavotti (1999).

Nonequilibrium Ensembles and Their Equivalence

Given a chaotic system, the collection of the SRB distributions associated with the various control parameters (volume, density, external forces,...) forms an "ensemble" describing the possible stationary states of the system and their statistical properties.

As in equilibrium, one can imagine that the system can be described equivalently in several ways at least when the system is large ("in the

thermodynamic" or "macroscopic limit"). In nonequilibrium, equivalence can be quite different and more structured than in equilibrium because one can imagine to change not only the control parameters but also the thermostatting mechanism.

It is intuitive that a system may behave in the same way under the influence of different thermostats: the important phenomenon being the extraction of heat and not the way in which it is extracted from the system. Therefore, one should ask when two systems are "physically equivalent," that is, when the SRB distributions associated with them give the same statistical properties for the same observables, at least for the very few observables which are macroscopically relevant. The latter may be a few more than the usual ones in equilibrium (temperature, pressure, density, etc.) and include currents, conducibilities, viscosities, etc., but they will always be very few compared to the (infinite) number of functions on phase space.

As an example, consider a system of N interacting particles (say hard spheres) of mass m moving in a periodic box C_0 of side L containing a regular array of spherical scatterers (a basic model for electrons in a crystal) which reflect particles elastically and are arranged so that no straight line exists in C_0 which avoids the obstacles (to eliminate obvious constants of motion). An external field $E\boldsymbol{u}$ acts also along the $\boldsymbol{u}$-direction: hence, the equations of motion are

$$m\ddot{x}_i = f_i + E\boldsymbol{u} - \boldsymbol{\vartheta}_i \qquad [20]$$

where f_i are the interparticle forces and those between scatterers and particles, and $\boldsymbol{\vartheta}_i$ are the thermostatting forces. The following thermostat models have been considered:

1. $\boldsymbol{\vartheta}_i = \nu\dot{x}_i$ (viscosity thermostat),
2. immediately after elastic collision with an obstacle the velocity is rescaled to a prefixed value $\sqrt{3k_{\rm B}Tm^{-1}}$ for some T (Drude's thermostat),
3. $\boldsymbol{\vartheta}_i = (\boldsymbol{E} \cdot \sum \dot{x}_i)/\sum_i \dot{x}_i^2$ (Gauss' thermostat).

The first two are not reversible. At least not manifestly such, because the natural time reversal, that is, change of velocity sign, is not a symmetry (there might be however more hidden, hitherto unknown, symmetries which anticommute with time evolution). The third is reversible and time reversal is just the change of the velocity sign. The third thermostat model generates a time evolution in which the total kinetic energy K is constant.

Let $\mu'_\nu, \mu''_T, \mu'''_K$ be the SRB distributions for the system in a container C_0 with volume $|C_0| = L^3$ and density $\rho = N/L^3$ fixed. Imagine to tune the values of the control parameters ν, T, K in such a way that $\langle\text{kinetic energy}\rangle_\mu = \mathcal{E}$, with the same $\mathcal{E}$ for $\mu = \mu'_\nu, \mu''_T, \mu'''_K$ and consider a local observable $F(\dot{\boldsymbol{X}}, \boldsymbol{X}) > 0$ depending only on the coordinates of the particles located in a region $\Lambda \subset C_0$. Then a reasonable conjecture is that

$$\lim_{\substack{L\to\infty \\ N/L^3=\rho}} \frac{\langle F\rangle_{\mu'_\nu}}{\langle F\rangle_{\mu''_T}} = \lim_{\substack{L\to\infty \\ N/L^3=\rho}} \frac{\langle F\rangle_{\mu'_\nu}}{\langle F\rangle_{\mu'''_T}} = 1 \qquad [21]$$

if the limits are taken at fixed F (hence at fixed Λ while $L \to \to \infty$). The conjecture is an open problem: it illustrates, however, the kind of questions arising in nonequilibrium statistical mechanics.

For more details, the reader is referred to Evans and Sarman (1993), Gallavotti (1999), and Ruelle (2000).

Outlook

The subject is (clearly) at a very early stage of development.

1. The theory can be extended to stochastic thermostats quite satisfactorily, at least as far as the fluctuation theorem is concerned.
2. Remarkable works have appeared on the theory of systems which are purely Hamiltonian and (therefore) with thermostats that are infinite: unfortunately, the infinite thermostats can be treated, so far, only if their particles are "free" at infinity (either free gases or harmonic lattices).
3. The notion of entropy turns out to be extremely difficult to extend to stationary states and there are even doubts that it could be actually extended. Conceptually, this is certainly a major open problem.
4. The statistical properties of stationary states out of equilibrium are still quite mysterious and surprising: some exactly solvable models have appeared recently, and attempts have been made at unveiling the deep reasons for their solubility and at deriving from them general guiding principles.
5. Numerical simulations have given a strong impulse to the subject; in fact, one can even say that they created it: introducing the model of thermostat as an extra microscopic force acting on the particles and providing the first reliable results on the properties of systems out of equilibrium. Simulations continue to be an essential part of the effort of research on the field.
6. Approach to stationarity leads to many important questions: is there a Lyapunov function measuring the distance between an evolving state and the stationary state towards which it evolves? In other words, can one define an

analogous of Boltzmann's H-function? About this question there have been proposals and the answer seems affirmative, but it does not seem that it is possible to find a universal, system-independent, such function (search for it is related to the problem of defining an entropy function for stationary states: its existence is at least controversial, see the sections "Nonequilibrium thermodynamics" and "Chaotic hypothesis").

7. Studying nonstationary evolution is much harder. The problem arises when the control parameters (force, volume,...) change with time and the system "undergoes a process." As an example one can ask the question of how irreversible is a given irreversible process in which the initial state μ_0 is a stationary state at time $t=0$, and the external parameters $\mathbf{\Phi}_0$ start changing into functions $\mathbf{\Phi}(t)$ of t and tend to a limit $\mathbf{\Phi}_\infty$ as $t \to \infty$. In this case, the stationary distribution μ_0 starts changing and becomes a function μ_t of t which is not stationary but approaches another stationary distribution μ_∞ as $t \to \infty$. The process is, in general, irreversible and the question is how to measure its "degree of irreversibility": for simplicity we restrict attention to very special processes in which the only phenomenon is heat production because the container does not change volume and the energy also remains constants, so that the motion can be described at all times as taking place on a fixed energy surface. A natural quantity $\mathcal{I}$ associated with the evolution from an initial stationary state to a final stationary state through a change in the control parameters can be defined as follows. Consider the distribution μ_t into which μ_0 evolves in time t, and consider also the SRB distribution $\mu_{\mathbf{\Phi}(t)}$ corresponding to the control parameters "frozen" at the value at time t, that is, $\mathbf{\Phi}(t)$. Let the phase-space contraction, when the forces are "frozen" at the value $\mathbf{\Phi}(t)$, be $\sigma_t(x) = \sigma(x; \mathbf{\Phi}(t))$. In general $\mu_t \neq \mu_{\mathbf{\Phi}(t)}$. Then,

$$\mathcal{I}(\{\mathbf{\Phi}(t)\}, \mu_0, \mu_\infty) \stackrel{\text{def}}{=} \int_0^\infty (\mu_t(\sigma_t) - \mu_{\mathbf{\Phi}(t)}(\sigma_t))^2 \, dt \qquad [22]$$

can be called the degree of irreversibility of the process: it has the property that in the limit of infinitely slow evolution of $\mathbf{\Phi}(t)$, for example, if $\mathbf{\Phi}(t) = \mathbf{\Phi}_0 + (1 - e^{-\gamma\kappa t})\Delta$ (a quasistatic evolution on timescale $\gamma^{-1}\kappa^{-1}$ from $\mathbf{\Phi}_0$ to $\mathbf{\Phi}_\infty = \mathbf{\Phi}_0 + \Delta$), the irreversibility degree $\mathcal{I}_\gamma \xrightarrow[\gamma \to 0]{} 0$ if (as in the case of Anosov evolutions, hence under the chaotic hypothesis) the approach to a stationary state is exponentially fast at fixed external forces $\mathbf{\Phi}$. The quantity $\mathcal{I}$ is a time scale which could be interpreted as the time needed for the process to exhibit its irreversible nature.

The entire subject is dominated by the initial insights of Onsager on classical nonequilibrium thermodynamics, which concern the properties of the infinitesimal deviations from equilibrium (i.e., averages of observables differentiated with respect to the control parameters $\mathbf{\Phi}$ and evaluated at $\mathbf{\Phi} = 0$). The present efforts are devoted to studying properties at $\mathbf{\Phi} \neq 0$. In this direction, the classical theory provides certainly firm constraints (like Onsager reciprocity or Green–Kubo relations or fluctuation–dissipation theorem) but at a technical level, it gives little help to enter the terra incognita of nonequilibrium thermodynamics of stationary states.

For more details, the reader is referred to Kurchan (1998), Lebowitz and Spohn (1999), Maes (1999), Eckmann *et al.* (1999), Bonetto *et al.* (2000, 2005), Eckmann and Young (2005), Derrida *et al.* (2001), Bertini *et al.* (2001), Evans and Morriss (1990), Evans *et al.* (1993), Goldstein and Lebowitz (2004), and Gallavotti (2004).

See also: Adiabatic Piston; Chaos and Attractors; Ergodic Theory; Lie, Symplectic, and Poisson Groupoids and Their Lie Algebroids; Macroscopic Fluctuations and Thermodynamic Functionals; Nonequilibrium Statistical Mechanics: Dynamical Systems Approach; Quantum Dynamical Semigroups; Random Dynamical Systems.

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Nonequilibrium Statistical Mechanics: Dynamical Systems Approach

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Time Evolution of Infinite-Particle Systems

A preliminary problem in the rigorous study of nonequilibrium statistical mechanics is to give a precise sense to the time evolution of infinitely extended systems. In fact, statistical mechanics deals with systems composed by a very large number of bodies (of the order of 10^{23}) and studies the properties of such systems which are related to their large number of degrees of freedom. Mathematically, this aspect is stressed by introducing the so-called "thermodynamical limit," that is, by defining and analyzing systems with infinite degrees of freedom. For particle systems, the problem can be formulated in the following way. A phase point of the system is an infinite sequence $\{(x_i, v_i)\}_{i\in\mathbb{N}}$ of the positions and velocities of the particles, and its time evolution is characterized by the solutions of the Newton equations:

$$m\ddot{x}_i(t) = \sum_{j\in\mathbb{N}:j\neq i} F\big(x_i(t) - x_j(t)\big), \quad i \in \mathbb{N} \qquad [1]$$

where m is the mass of each particle, $F(x) = -\nabla\Phi(x)$, and Φ is a two-body potential. Equation [1] must be completed by the initial data $\{(x_i(0), v_i(0))\}_{i\in\mathbb{N}}$. The time evolution of a phase point implies in a natural way the time evolution of functions on the phase space, which are the observables to be compared with experiments.

The existence of a solution to eqn [1] is not obvious, because the classical theorem of existence and uniqueness for the Cauchy problem of the Newton equations depends on the number of degrees of freedom of the system. The main difficulty is that *a priori* the time evolution can bring infinitely many particles in a bounded region within a finite time, so that the right-hand side of eqn [1] becomes meaningless. Without any hypothesis on the initial conditions, this can happen, as shown by the following simple example. Consider a system of free (noninteracting) particles moving on the real line with initial conditions $x_i = i$, $v_i = -i$, $i \in \mathbb{N}$. It is clear that at time $t = 1$ all the particles are at the origin. To forbid this "collapse," we must restrict the allowed initial conditions, but we cannot be too drastic. For instance, we could surely avoid these pathologies by choosing the initial velocities uniformly bounded and the initial distribution of particles locally finite. But the set of such data is exceptional with respect to the Gibbs state (as it can be easily shown using that, at equilibrium, the velocities are independent identically distributed Gaussian variables). In conclusion, we must construct the dynamics for initial conditions which are chosen in a set sufficiently large to

be the support of states of interest from a thermodynamical point of view.

The difficulty of the problem increases with the spatial dimension d, as it is shown by the following example. Let the potential Φ be smooth enough and short range and assume that, initially, the velocities and the density are bounded, that is,

$$\sup_i |\boldsymbol{v}_i| < \infty, \qquad \sup_{\mu \in \mathbb{R}^d, R>1} \frac{N(X;\mu,R)}{R^d} < \infty \qquad [2]$$

where $X = \{(\boldsymbol{x}_i, \boldsymbol{v}_i)\}_{i\in\mathbb{N}}$ is the particle configuration and $N(X;\mu,R)$ is the number of particles in the ball of radius R, centered at μ. If $V(t)$ denotes the modulus of the maximal velocity carried by the particle during the time $[0,t]$ and $X(t)$ the evolved configuration, the conservation of the particles number yields

$$N(X(t);\mu,R_0) \le N(X(0);\mu,R(t)) \le \text{const.}\, R(t)^d \qquad [3]$$

where

$$R(t) = R_0 + \int_0^t \mathrm{d}s V(s) \qquad [4]$$

On the other hand, $V(s)$ is controlled by the force, which turns out to be bounded by $\sup_\mu N(X(s);\mu,r)$, where $r > 0$ is the range of the potential. By virtue of eqns [3] and [4], we arrive at the integral inequality:

$$R(t) \le R_0 + \text{const.}\, t + \text{const.} \int_0^t \mathrm{d}s R(s)^d \qquad [5]$$

which is solvable globally in time only if $d = 1$.

In the case of interest, from a thermodynamical point of view, we also need to allow fluctuations of the density and velocities, which add further difficulties. The existence, uniqueness, and locality of the motion has been solved in dimension $d = 1$ for almost all relevant interactions (Lanford 1968, Dobrushin and Fritz 1977), and in dimension $d = 2$ for interactions not too singular at the origin (Fritz and Dobrushin 1977). (This does not cover, for instance, the hard-core interactions, where it is still an open problem to investigate whether the dynamics evolves toward a close-packing situation.) Finally, in dimension $d = 3$, the result has recently been proved only for bounded, non-negative, finite-range interactions (Caglioti *et al.* 2000).

We state the result for the three-dimensional case. Let the interaction Φ depend only on the mutual distance, be twice differentiable, positive in the origin and, for the moment, also non-negative and compactly supported. We assume that the initial data have bounded local energies and densities, with at most logarithmic divergences in velocities and densities. More precisely, we define

$$Q(X;\mu,R) = \sum_{i\in\mathbb{N}} \chi(|\boldsymbol{x}_i - \mu| \le R) \times \left[\frac{m\boldsymbol{v}_i^2}{2} + \frac{1}{2}\sum_{j:j\neq i} \Phi(\boldsymbol{x}_i - \boldsymbol{x}_j) + 1\right] \qquad [6]$$

where $\chi(A)$ denotes the characteristic function of the set A so that eqn [6] gives the energy and density contained in a ball centered at μ with radius R. Define

$$Q_\alpha(X) = \sup_\mu \sup_{R:R>\phi_\alpha(\mu)} \frac{Q(X;\mu,R)}{R^3} \qquad [7]$$

where $\alpha > 0$ and

$$\phi_\alpha(\boldsymbol{x}) \doteq \log^\alpha(e + |\boldsymbol{x}|), \quad \boldsymbol{x} \in \mathbb{R}^3 \qquad [8]$$

We denote by $\mathcal{X}_\alpha$ the set of the phase points X such that $Q_\alpha(X) < \infty$. It is possible to prove that for any $\alpha \ge 1/3, \mathcal{X}_\alpha$ has full measure with respect to any Gibbs measure.

We define the partial dynamics $t \mapsto X^{(n)}(t)$ as the solutions to eqn [1] obtained by neglecting all the particles which are initially outside the ball of radius n and centered at the origin.

Theorem *If $X \in \mathcal{X}_\alpha$ there exists a unique flow $X \to X(t) \in \mathcal{X}_{(3/2)\alpha}$ satisfying eqn* [1] *with $X(0) = X$. Moreover, the partial dynamics locally converges to $X(t)$ as $n \to \infty$.*

The result has been extended to bounded superstable long-range interactions. The (nontrivial) proof is based on several steps: we introduce a mollified version on the local energy and study its evolution in time under the partial dynamics. The energy conservation allows us to prove that the local energy grows at most as the cube of the maximal velocity. On the other hand, a suitable time average allows us to control the maximal velocity via the local energy in an appropriate way. The result is achieved by letting $n \to \infty$.

Long-Time Behavior

Existence and locality of the dynamics is only a first, preliminary, step. The next and much more subtle question concerns the asymptotic (in time) and the statistical properties of the motion. Here, the main problem is the absence of simple but nontrivial models. Let us explain this point by a comparison with the situation in equilibrium statistical mechanics. In this case, even the simpler model, the free-particle system, exhibits all the relevant

thermodynamical properties of real systems away from the critical regime. In fact, the effort is often reduced to rigorously proving that the real systems away from the critical region behave as a free-particle system. The presence of the interaction is instead essential to describe phase transitions.

In the case of nonequilibrium statistical mechanics there are very few solvable models (free particles, chain of oscillators, hard-core system in one dimension), and typically they do not catch the essential properties of the real systems. For example, let us consider a system which is close to equilibrium and ask whether it converges to the corresponding Gibbs state. Two possible mechanisms usually come together: the dispersive properties of the matter (by which perturbations "escape" to infinity) and the mixing properties (by which perturbations are "spread" and disappear). The former is present also in the free-particle system, being responsible of its ergodic properties. The latter requires a deep analysis of the dynamics of interacting-particle systems and it is too difficult to be analyzed except in rare cases.

We just mention the case of systems with instantaneous interaction, which are simple enough to be studied but nevertheless exhibit a nontrivial long-time behavior. We recall in particular the famous Sinai's billiard: a particle moving freely in a two-dimensional torus except for elastic collisions with the boundary of a convex obstacle. As proved by Sinai (1970), this system has strong ergodic properties. Sinai's billiard can be proved to be equivalent to the "Lorentz gas" in which the obstacles are dislocated in a periodic way. Bunimovich and Sinai (1981) proved that when the obstacles are close enough to each other, the diffusive (weak) limit of the particle motion is the Wiener process. This remarkable result gives a rigorous derivation of Brownian motion from a Hamiltonian system.

More recently, similar questions have been investigated in the case of a charged particle subject to a constant electric field and interacting with a medium described by a particle system. Several rigorous results have been obtained on this subject. We only recall those by Boldrighini and Soloveitchik (1995, 1997). In the context of a simplified model, the asymptotic motion of the charged particle is described as a drift plus a Brownian motion, and the Einstein relation between the drift and the diffusion constant is established.

Mean-Field Limit

The validity of any model is related to some approximation limit. In statistical mechanics, we encounter one of the most important ones, the "thermodynamical limit," used to stress the effect of large number of particles. Here we briefly discuss the "mean-field limit." For the kinetic, Boltzmann–Grad limit, *see* Boltzmann Equation (Classical and Quantum) and Kinetic Equations.

We consider N particles of mass m mutually interacting via the force $\boldsymbol{F}$. The equations of motion are

$$\begin{cases} m\ddot{\boldsymbol{x}}_i(t) = \sum_{j=1,\dots,N: j\neq i} \boldsymbol{F}(\boldsymbol{x}_i(t) - \boldsymbol{x}_j(t)) \\ (\boldsymbol{x}_i(0), \dot{\boldsymbol{x}}_i(0)) = (\boldsymbol{x}_i, \boldsymbol{v}_i) \end{cases} \quad i = 1, \dots, N \qquad [9]$$

We consider a system with N very large, the mass m of each particle very small, and the interaction very weak. An interesting situation arises when the quantities N, m, and $\boldsymbol{F}$ are linked by the relations

$$m = \frac{M}{N}, \qquad \boldsymbol{F} = \frac{\boldsymbol{G}}{N^2} \qquad [10]$$

for some function $\boldsymbol{G}$. Of course, M is the total mass of the system.

We are interested in investigating the limit $N \to \infty$. We assume that the initial data are chosen in a way that the empirical measure $N^{-1}\sum_i \delta_{\boldsymbol{x}_i}\delta_{\boldsymbol{v}_i}$ weakly converges (as $N \to \infty$) to the absolutely continuous measure $f_0(\boldsymbol{x}, \boldsymbol{v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$ with some smooth density $f_0(\boldsymbol{x}, \boldsymbol{v})$. We ask whether at some positive time $t > 0$ the empirical measure $N^{-1}\sum_i \delta_{\boldsymbol{x}_i(t)}\delta_{\boldsymbol{v}_i(t)}$ weakly converges to $f(\boldsymbol{x}, \boldsymbol{v}, t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$ with a density $f(\boldsymbol{x}, \boldsymbol{v}, t)$ satisfying some limiting evolution equation.

Formally, it is easy to find this equation: by the Liouville theorem, a continuous medium in which each point moves under the action of an acceleration field behaves as an incompressible fluid. The continuity equation becomes

$$\begin{gathered} \partial_t f(\boldsymbol{x}, \boldsymbol{v}, t) + \boldsymbol{v} \cdot \nabla_x f(\boldsymbol{x}, \boldsymbol{v}, t) + \boldsymbol{E} \cdot \nabla_v f(\boldsymbol{x}, \boldsymbol{v}, t) = 0 \\ f(\boldsymbol{x}, \boldsymbol{v}, 0) = f_0(\boldsymbol{x}, \boldsymbol{v}) \end{gathered} \qquad [11]$$

where

$$\boldsymbol{E}(\boldsymbol{x}, t) = \int_{\mathbb{R}^3} \mathrm{d}\boldsymbol{y}\, \boldsymbol{G}(\boldsymbol{x} - \boldsymbol{y})\rho(\boldsymbol{y}, t) \qquad [12]$$

$$\rho(\boldsymbol{x}, t) = \int_{\mathbb{R}^3} \mathrm{d}\boldsymbol{v}\, f(\boldsymbol{x}, \boldsymbol{v}, t) \qquad [13]$$

This equation can be studied by following the characteristics, for which it suffices to look at the pair of functions

$$(\boldsymbol{x}, \boldsymbol{v}) \mapsto (\boldsymbol{X}(\boldsymbol{x}, \boldsymbol{v}, t), \boldsymbol{V}(\boldsymbol{x}, \boldsymbol{v}, t)), \qquad f_0(\boldsymbol{x}, \boldsymbol{v}) \mapsto f(\boldsymbol{x}, \boldsymbol{v}, t)$$

where $(x, v) \in \mathbb{R}^3 \times \mathbb{R}^3$ and $t \in \mathbb{R}$, solutions of

$$\begin{aligned} &\dot{X}(x,v,t) = V(x,v,t),\ \dot{V}(x,v,t) = E(x,t) \\ &X(x,v,0) = x,\ V(x,v,0) = v \\ &f(X(x,v,t), V(x,v,t), t) = f_0(x,v) \end{aligned} \quad [14]$$

This is a weak formulation of eqn [11], in the sense that any smooth solution to eqn [11] satisfies eqn [14], but this last equation in meaningful also for nonsmooth functions. This is a weak version of the Vlasov equation and its measure solutions will play an important role in the sequel.

Equations [11]–[14] are called Vlasov equations, after Vlasov, who first introduced them in plasma physics. They have a Hamiltonian structure and conserve several quantities: the total mass, the total energy, the Liouville measure $\mathrm{d}x\,\mathrm{d}v$, and in general each moment of this measure.

The existence and uniqueness of the solutions has been studied in many papers. Two cases have to be considered, depending on whether the total mass

$$M = \int_{\mathbb{R}^6} \mathrm{d}x\,\mathrm{d}v\, f_0(x,v) \quad [15]$$

is finite or not. We start with the first case. If the interaction G is bounded, the analysis is easy. On the other hand, in plasma physics one deals with the Coulomb interaction, which is singular at the origin. In this case (where eqn [11] is usually called the Vlasov–Poisson equation), existence and uniqueness can still be proved, but it is not straightforward, especially in dimension $d=3$. The case with the complete Lorentz force, also taking into account the relativistic effect, is much more difficult.

For infinite total mass, the problem has been solved recently in three (or lower) dimensions for bounded, non-negative, finite-range interactions, and in two dimensions for singular Helmholtz interactions.

Another way to relate the Vlasov equation with the particle systems is to consider the usual transition from microscopic to macroscopic evolutions based on a separation between microscopic and macroscopic scales. Moreover, the force between the particles is due to a long-range pair interaction of the Kac type, in which the range parameter tends to infinity as the ratio ε^{-1} between the macro and the micro spatial scale: $F(x_i - x_j) = \varepsilon^{2d+1} G(\varepsilon x_i - \varepsilon x_j)$. Finally, the mass of the particles is proportional to ε^d: $m = \varepsilon^d$. After rescaling space and time by a factor ε, in the macroscopic variables $(\tau, r) = (\varepsilon t, \varepsilon x)$, the equations of motion (eqn [9]) become

$$\frac{\mathrm{d}r_i}{\mathrm{d}\tau^2} = \sum_{j:j\neq i} \varepsilon^d G(r_i - r_j) \quad [16]$$

Then eqn [14] is the limiting equation as $\varepsilon \to 0$.

Other Models

We mention another model of larger interest. We introduce it in the simplest formulation, leaving possible generalizations to the reader.

We consider an infinite chain of anharmonic oscillators, with Hamiltonian H given by

$$H(q,p) = \sum_{i\in\mathbb{Z}} \left[\frac{p_i^2}{2m} + a q_i^4 + b \sum_{j:|i-j|=1} (q_i - q_j)^2 + c q_i^2 + d \right] \quad [17]$$

where $q_i, p_i \in \mathbb{R}$, $a \geq 0$, $b, c, d > 0$.

When $a = 0$, it reduces to the well-known chain of harmonic oscillators, which is integrable and widely studied in the literature.

The time evolution defined by the Hamiltonian in eqn [17] exists and it is unique for initial data chosen in a set large enough to be the support of any reasonable thermodynamic (equilibrium or nonequilibrium) state. This can be achieved by proving integral inequalities for the "Lyapunov function"

$$L(q,p) = \sup_{i\in\mathbb{Z}} \left[\frac{p_i^2}{2m} + a q_i^4 + d \right] \frac{1}{|i|+1}$$

It is interesting to note that uniqueness holds only in a class of data such that the position of the ith oscillator does not increase too much as $|i| \to \infty$. For example, besides the stationary solution $q_i(t) = 0, i \in \mathbb{Z}$, we can construct a different solution corresponding to the same initial conditions $q_i(0) = 0$, $p_i(0) = 0$, $i \in \mathbb{Z}$. In fact, by imposing $q_0(t) = t^2$ and $q_i(t) = q_{-i}(t)$, we can solve recursively the equations of motion and obtain a nonzero solution $q_i(t)$, which however increases superexponentially as $|i| \to \infty$.

The Hamiltonian dynamical systems (classical or quantum) are surely quite faithful descriptions of real systems, but they are too difficult to study. Mainly it is not known how to prove good dynamical mixing for deterministic evolutions with many degrees of freedom. Therefore, stochastic evolutions have been introduced to model the real systems. More precisely, one renounces a full description of the microscopic dynamics, introducing simplified models where the effects of the

"hidden degrees of freedom" are taken into account by adding suitable stochastic forces. Many useful results have been obtained, which show that these stochastic model systems exhibit a macroscopic behavior much closer to that observed in nature. The main criticism concerns the role of stochasticity, which in these models is introduced *ab initio*. In other words, if one believes that the statistical properties of the deterministic motion on the small scale determine the collective behavior of systems with many degrees of freedom, then these properties do have to be proved for a true understanding of nonequilibrium phenomena.

See also: Adiabatic Piston; Boltzmann Equation (Classical and Quantum); Fourier Law; Kinetic Equations; Nonequilibrium Statistical Mechanics (Stationary): Overview; Nonequilibrium Statistical Mechanics: Interaction between Theory and Numerical Simulations.

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Nonequilibrium Statistical Mechanics: Interaction between Theory and Numerical Simulations

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Introduction

Nonequilibrium statistical mechanics concerns a wide range of fundamental problems and applications. Perturbative methods are quite effective for approaching weakly nonlinear problems, usually relying upon effective coarse-grained equations. The attempt of obtaining a microscopic description of genuine nonlinear problems demands the combined use of theoretical methods and numerical simulations. The proprotypic case is the numerical experiment performed by Fermi, Pasta, and Ulam in 1955. As we discuss in the following section, the main questions, which had inspired this experiment, remained without an answer for a long time, while new puzzling problems emerged. Despite its apparent failure, the Fermi–Pasta–Ulam (FPU) experiment represents a remarkable example in the history of science of how a good guess may be the source of many fruitful achievements. Part of them are discussed in the section on energy relaxation in nonlinear chains, where we summarize the present understanding of the very slow relaxation mechanism, characterizing the dynamics of nonlinear chains of oscillators, like the FPU model, at low energies. Next, we report one further success of the interplay between theory and numerics, that is, the formulation of a generalized fluctuation–dissipation relation for stationary processes. Finally, we survey the main achievements concerning the study of anomalous transport properties in low-dimensional systems. In particular, we focus our attention on the heat conduction in nonlinear lattices. Lacking a general hydrodynamic theory, also in this case computer simulations and theoretical arguments have greatly

contributed to clarify the general scenario, unveiling surprising aspects, which, up to a few years ago, were completely unexpected.

The Numerical Experiment by Fermi, Pasta, and Ulam

The impressive progress of electronic technology during World War II made possible the design of the first digital computers. The equally impressive budgets for their production and maintenance could only be justified by their employment in classified military research. Nonetheless, some of the outstanding scientists involved in these researches, like E Fermi, immediately realized the great potential of these new machines for tackling also some fundamental problems in basic science.

Fermi had in his mind a crucial and still open physical problem. In 1914 the Dutch physicist P Debye had suggested that the finiteness of thermal conductivity in crystals should be due to the nonlinear forces acting among the constituent atoms. Forty years later a microscopic theory of transport processes, including nonlinear effects, was still lacking. Actually, technical difficulties prevented a theoretical approach based on analytic methods. Numerical integration of the equations of motion by a digital machine appeared to Fermi as an effective way for tackling this problem. In collaboration with the mathematician S Ulam and the physicist J Pasta, Fermi used MANIAC 1 (a prototype digital computer installed at Los Alamos National Laboratories, USA) for integrating the dynamical equations of the simplest mathematical model of an anharmonic crystal: a chain of N harmonic oscillators, coupled by nonlinear forces. Its Hamiltonian reads

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{\omega^2}{2}(q_{i+1} - q_i)^2 + \frac{\alpha}{3}(q_{i+1} - q_i)^3 + \frac{\beta}{4}(q_{i+1} - q_i)^4 \qquad [1]$$

where ω is the harmonic frequency, while α and β are the positive coupling constants of the nonlinear terms. The integer space index i labels the oscillators along the chain, while q_i and p_i are the displacement from the equilibrium position and the momentum of the ith oscillator, respectively. The potential energy is the general form taken by any nonlinear interaction potential, when expanded, up to fourth order, around its equilibrium position. This choice guarantees the boundedness of trajectories for any finite energy.

Accordingly, the model contains the minimal basic ingredients, needed for testing the conjecture about the finiteness of thermal conductivity.

The equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad [2]$$

were integrated numerically by an algorithm, where space and time derivatives were approximated by proper finite-difference expressions.

The choice of the initial conditions was motivated by a further basic question concerning Fermi and his collaborators. In fact, they aimed at verifying also a common belief that had never been proved rigorously: in an isolated mechanical system with many degrees of freedom (i.e., made of a large number of oscillators), a generic nonlinear interaction among them should eventually yield equilibrium through "thermalization" of the energy. On the basis of physical intuition, nobody would object to this expectation if the mechanical system would start its evolution from an initial state very close to thermodynamic equilibrium. Nonetheless, the same should be observed by considering an initial state, where energy is supplied to a small subset of oscillatory modes of the crystal. At variance with a finite system of linear oscillators, where each initially excited mode keeps its energy constant, nonlinear terms should make the energy flow towards all oscillatory modes, until thermal equilibrium is eventually reached. Thermalization corresponds to energy equipartition among all the modes. This statement has to be interpreted in a statistical sense: the time averages of the energies contained in the modes converge to the same constant value. But if this was the case, one further fundamental aspect concerning the evolution towards thermodynamic equilibrium could be checked. In the formulation of his transport equation, L Boltzmann had conjectured that thermodynamic irreversibility can emerge from microscopic reversible dynamics (which is the case of eqns [2]). The paradoxical implication of Boltzmann's conjecture was pointed out by H Poincaré, who had proved that any isolated Hamiltonian system necessarily evolves towards an almost-recurrent dynamics. This is manifestly incompatible with the second law of thermodynamics, which implies that thermodynamic systems, in the absence of a supplied energy flux, have to evolve irreversibly towards their equilibrium state. In this perspective, the FPU numerical experiment was intended to test also if and how equilibrium is approached by a relatively large number of nonlinearly coupled oscillators, obeying the classical

laws of Newtonian mechanics. Furthermore, the measurement of the time interval needed for approaching the equilibrium state, that is, the "relaxation time" of the chain of oscillators, would have provided an indirect determination of thermal conductivity. In fact, according to elementary kinetic theory, the relaxation time, τ_r, represents an estimate of the timescale of energy exchanges inside the crystal: Debye's argument predicts that thermal conductivity κ is proportional to the specific heat at constant volume of the crystal, C_v, and inversely proportional to τ_r, in formulas $\kappa \propto C_v/\tau_r$.

Fermi, Pasta, and Ulam considered relatively short chains, up to 64 oscillators – a size that already challenged the limits of the computational power of MANIAC 1. They imposed fixed boundary conditions (i.e., the particles at the chain boundaries interact with infinite mass walls) and the energy was initially stored just in one of the long-wavelength oscillatory modes.

A very surprising and unexpected scenario showed up. Contrary to any intuition, the energy did not flow to the higher modes, but was exchanged only among a small number of long-wavelength modes, before flowing back almost exactly to the initial state, thus yielding a recurrent behavior.

Although nonlinearities were at work, neither a tendency towards thermalization, nor a mixing rate of the energy could be identified. The dynamics exhibited regular features very close to those of an integrable system.

Fermi guessed that they were facing a very important result, but he was also quite disappointed by the difficulties in finding a convincing explanation. This lacking, he had decided not to publish the results in a scientific review, which remained confined into a Los Alamos report for almost one decade. In fact, he died in 1955, the same year of publication of the report.

The results were finally published in 1965, in a volume containing his collected papers (Fermi *et al.* 1965), and they immediately raised a renewed interest in the scientific community. Despite the failure in answering all the questions that had been raised, the FPU numerical experiment represents a crucial scientific achievement, which determined many subsequent scientific progresses. The implications about nonequilibrium will be widely discussed in the following sections. Here, we want to conclude by mentioning the important developments, inspired by the FPU experiment, that led to the discovery of solitons by Zabusky and Kruskal in 1965.

Slow and Fast Energy Relaxation in Nonlinear Chains

The results of the FPU numerical experiment indicate that the energy initially supplied to long-wavelength oscillatory (Fourier) modes remains localized for a very long time in a small subset of long-wavelength modes. This time can be exceedingly larger than any typical timescale of the model (e.g., ω^{-1}, i.e., the inverse of the harmonic frequency in [1]). An explanation of this apparently bizarre scenario has been tackled by combining theoretical approaches with numerical studies. A complete account of the many contributions in this direction being beyond the scope of this text, we shall summarize the two main lines along which this problem has been considered.

The Resonance-Overlap Criterion

The almost-recurrent behavior of single-mode excitations studied in the FPU experiment can be explained by the resonance-overlap criterion, introduced in 1959 by the Russian scientist B Chirikov. Moreover, this criterion provides a quantitative estimate of the value of the energy density, above which the regular motion observed in the FPU experiment should be definitely lost.

In order to provide the reader with an illustration of this criterion, we have to introduce a few simple mathematical ingredients.

The Hamiltonian [1] can be rewritten in terms of linear normal Fourier coordinates, $(Q_k(t), P_k(t))$, as follows:

$$H = \frac{1}{2}\sum_k (P_k^2 + \omega_k^2 Q_k^2) + \alpha V_3(\{Q_k\}) + \beta V_4(\{Q_k\}) \qquad [3]$$

Here, we have used the shorthand notation $V_n(\{Q_k\})$ for the lengthy explicit expressions, in the new set of coordinates, of the nonlinear potentials of [1].

Without prejudice of generality, we can impose periodic boundary conditions to the FPU chain: the frequency of the kth normal mode is given by the expression $\omega_k = 2\sin(\pi k/N)$. The coupling constants α and β control the energy exchange among the normal modes, due to nonlinear interactions.

For the sake of space, we give here a brief sketch of Chirikov's criterion for the FPU β-model (this model amounts to take $\alpha = 0$ in [3], i.e., to exclude the cubic part of the nonlinear potential).

By making reference to the initial conditions of the FPU experiment, we can consider a single excited mode, so that the Hamiltonian [3] can be

approximated by the expression in action-angle variables

$$H = H_0 + \beta H_1 \approx \omega_k J_k + \frac{\beta}{2N}(\omega_k J_k)^2 \qquad [4]$$

Here, $J_k = \omega_k Q_k^2$ is the action variable. In practice, this amounts to approximate the original Hamiltonian by the sum of the harmonic and nonlinear self-energy of the initially excited mode. In this framework, H_0 and H_1 are the unperturbed (integrable) Hamiltonian and the perturbation, respectively. Indeed, if the energy is initially attributed to mode k, the following relations hold: $\omega_k J_k \approx H_0 \approx E$. By the approximated Hamiltonian [4], one can compute the nonlinear correction to the linear frequency ω_k, giving the renormalized frequency ω_k^{r}:

$$\omega_k^{\mathrm{r}} = \frac{\partial H}{\partial J_k} = \omega_k + \frac{\beta}{N}\omega_k^2 J_k = \omega_k + \Omega_k \qquad [5]$$

For $N \gg k$ one has

$$\Omega_k \approx \frac{\beta H_0 k}{N^2} \qquad [6]$$

The distance between two primary resonances, in the harmonic limit, is given by the expression

$$\Delta\omega_k = \omega_{k+1} - \omega_k \approx N^{-1} \qquad [7]$$

Consistently with [6], the last approximation is valid only for small wave number ($k \ll N$), that is, long-wavelength modes.

The "resonance overlap" criterion amounts to compare this distance with the frequency shift. In formulas:

$$\Omega_k \approx \Delta\omega_k \qquad [8]$$

This equation allows to obtain also an estimate of the "critical" energy density, ϵ_{c}, above which sizeable chaotic regions develop and a fast diffusion takes place in phase space:

$$\epsilon_{\mathrm{c}} = \left(\frac{H_0}{N}\right)_{\mathrm{c}} \approx \frac{1}{\beta k} \qquad [9]$$

with $k = O(1) \ll N$. Below ϵ_{c}, primary resonances are weakly coupled and determine a slow-relaxation process to energy equipartition. Above ϵ_{c}, due to "primary resonance" overlap, fast relaxation to equipartition sets in (Izrailev and Chirikov 1966).

This prediction was verified numerically later by Chirikov *et al.* (1973). The presence of a critical energy density can be tested by measuring the evolution of the finite time-averaged quantity $\bar{E}_k(t) = t^{-1}\int_0^t E_k(\tau)\mathrm{d}\tau$, where $E_k = (P_k^2 + \omega_k^2 Q_k^2)/2$ is the harmonic energy of the kth mode. For energy densities much smaller than ϵ_{c}, $\bar{E}_k(t)$ exhibits an extremely slow relaxation towards the equipartition condition, $\bar{E}_k =$ constant. Conversely, for $\epsilon > \epsilon_{\mathrm{c}}$ such a condition is rapidly approached on a relatively short timescale. The slow relaxation below ϵ_{c} can be traced back to the overlap of higher-order resonances: its typical timescale has been found to be inversely proportional to a power of the energy density (Shepelyansky 1997).

Energy-Equipartition Thresholds

The first paper reporting evidence of the existence of an energy threshold in chains of coupled anharmonic oscillators had already been published in 1970 by Bocchieri *et al.* (1970). This pioneering numerical experiment concerned a chain of oscillators coupled through a Lennard-Jones interatomic potential. The Italian group observed an energy threshold, separating a high-energy thermalized regime from a regular dynamics regime at low energies (like the one observed by Fermi, Pasta, and Ulam). The main point raised by this experiment concerns the consequences on ergodic theory: the ordered motion observed in the low-energy regime seems to violate ergodicity, although the model is known to be chaotic at any energy.

This is quite a delicate and widely debated issue for its statistical implications. Actually, as we have mentioned in the previous section, also Fermi, Pasta, and Ulam expected that a nonlinear dynamical system, made of a large number of degrees of freedom, should naturally evolve towards equilibrium. Further confirmations to the seminal paper by Bocchieri and co-workers came from more refined numerical experiments, showing that, for sufficiently high energies, regular behaviors disappear, while equipartition among the Fourier modes sets in rapidly. Later on, the presence of the energy threshold was characterized by introducing an appropriate entropy, $S = -\sum_k p_k \ln p_k$ with $p_k = \langle E_k(t)/E\rangle$, which counts the number of effective Fourier modes involved in the dynamics: at equipartition, this entropy is maximal (Livi *et al.* 1985).

Nowadays, we know that the approach to equipartition below and above the energy threshold is a matter of timescales, which turn out to be very different in the two regimes. For instance, the analytic estimate of the maximum Lyapunov exponent λ of the FPU β-model (Casetti *et al.* 1995) has definitely pointed out that there is a threshold value of the energy density, ϵ_{T}, at which its dependence on ϵ changes drastically:

$$\lambda(\epsilon) \sim \begin{cases} \epsilon^{1/4} & \text{if } \epsilon \gg \epsilon_{\mathrm{T}}; \\ \epsilon^2 & \text{if } \epsilon \ll \epsilon_{\mathrm{T}}. \end{cases} \qquad [10]$$

This implies that the typical relaxation time, that is λ^{-1}, may become exceedingly large for very small values of ϵ below ϵ_T. It is worth stressing that this result holds in the thermodynamic limit, thus indicating that the presence of ϵ_T is statistically relevant.

A more controversial scenario emerges from the studies of the relaxation dynamics for specific classes of initial conditions. When a few long-wavelength modes are initially excited, regular motion may persist over times much longer than λ^{-1} (De Luca *et al.* 1995). The excitation of small-wavelength modes yields an even more complex scenario: solitary wave dynamics is observed, followed by slow relaxation to equipartition. It is also worth mentioning that some regular features of the dynamics persist even at high energies. As we shall discuss in the section "Heat transport," such regularities still play a crucial role in determining energy transport mechanisms, although they do not affect significantly the equilibrium statistical properties of the FPU model at high energies.

The Generalized Fluctuation–Dissipation Theorem

Another fundamental problem of nonequilibrium statistical mechanics concerns the possibility of establishing a fluctuation–dissipation theorem, generalizing the relation valid for equilibrium conditions. In fact, on this basis one might develop a large-deviation formalism, aiming at the identification of an explicit nonequilibrium statistical measure, analogous to the equilibrium Boltzmann–Gibbs measure. Recently, some relevant progresses in this direction have been made.

A crucial numerical experiment, which attracted the attention on the problem of formulating a generalized fluctuation–dissipation relation for stationary flows, was performed at the beginning of the 1990s (Evans *et al.* 1993). Stationary conditions for momentum transport were obtained in the shear flow of a fluid contained between moving walls. The reversibility of the microscopic dynamics yields the heuristic fluctuation relation:

$$\frac{1}{t}\ln\frac{\Pr(\bar{R}_t = A)}{\Pr(\bar{R}_t = -A)} = -A \qquad [11]$$

where $\Pr(\bar{R}_t = A)$ is the probability that the average entropy production rate, $\bar{R}_t$, along a trajectory segment of duration t, takes the value A. For sufficiently large values of t, this relation was confirmed by numerical analysis.

Gallavotti and Cohen (1995a,b) proved a theorem meant to put on a rigorous mathematical basis eqn [11], that is, the proposed extension to nonequilibrium steady states of the equilibrium fluctuation–dissipation theorem. This theorem concerns the phase-space contraction rate of the dynamics, which equals the entropy production rate in the case of particle systems, whose internal energy is a constant of the motion. The proof of the theorem is based on restrictive hypotheses, which include the existence of an average non-vanishing phase-space contraction rate, the time-reversal invariance of the dynamics and a strong form of chaos (the dynamics is assumed to be of the Anosov type, that is, smooth and uniformly hyperbolic). Nonetheless, the prediction of the theorem, that is,

$$\frac{1}{t}\ln\frac{\Pi_t(p)}{\Pi_t(-p)} = D\langle\sigma\rangle p \qquad [12]$$

is expected to hold much more generally. Here $\Pi_t(p)$ is the probability that a fluctuation variable takes the value p. The theorem proved by Gallavotti and Cohen states that $\Pi_t(p)$ has to satisfy the large deviation relation [12], where σ is the average phase-space contraction rate over a trajectory segment of duration t and D is a suitable constant. It must be pointed out that the rigorous derivation of this relation provided strong motivations for investigating its validity and generality in many other contexts. The first numerical experiment, where almost all the constituent hypotheses of the Gallavotti–Cohen theorem were satisfied, was performed by Bonetto *et al.* (1997). They studied a Lorentz gas (massive pointlike noninteracting particles bouncing elastically on circular scatterers displaced on a regular lattice without free horizon) of charged particles moving in an uniform external electric field. Numerical simulations were found to be in very good agreement with [11] and [12] (which, in this case, refer to the same quantity). One further test of the fluctuation–dissipation relation was later performed for a different setup (Lepri *et al.* 1998). The FPU β-model is put in contact at its boundaries with thermal heat baths of different temperatures T_+ and $T_-(T_+ > T_-)$. Numerical simulations have been performed for sufficiently large applied thermal gradients, which guarantee sizeable effects of fluctuations, suitable for verifying a relation like [11]. It is worth noticing that many of the constituent hypotheses of the Gallavotti–Cohen theorem are not valid for this setup, but eqn [12] is still expected to hold, although in this case it does not refer to the entropy production rate. Nonetheless, the extension [11] of the fluctuation–dissipation theorem can be tested, thanks to the following useful relation,

between the heat flux j and the entropy production rates, $\zeta_\pm$, at the chain boundaries:

$$\langle \zeta_+ \rangle + \langle \zeta_- \rangle = j\left(\frac{1}{T_-} - \frac{1}{T_+}\right) \qquad [13]$$

This can be interpreted as a balance relation for the global entropy production. In fact, according to the principles of irreversible thermodynamics, the local rate of entropy production σ in the bulk is given by

$$\sigma(x) = j\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{T(x)}\right) \qquad [14]$$

By integrating this equation, one straightforwardly obtains the previous one, which then applies to the entropy production from the heat baths. Careful numerical simulations show that stationary conditions are found to hold over a wide range of temperatures and gradients. Equation [13] indicates that the heat flux is equivalent to the entropy production rate, apart from a multiplicative constant which depends on the amplitude of the applied field.

Let us define the finite-time average of the global heat flux

$$J_t = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{t}\int_0^t \mathrm{d}\tau j_i(\tau) \qquad [15]$$

The normalization of this quantity can be obtained by computing the asymptotic average value

$$J_\infty = \lim_{t\to\infty} J_t \qquad [16]$$

The quantity of statistical interest is the normalized finite-time average global heat flux

$$z = \frac{J_\tau}{J_\infty} \qquad [17]$$

Accordingly, the fluctuation–dissipation relation in this case takes the form:

$$\ln\frac{P_\tau(z)}{P_\tau(-z)} = \tau z j\left(\frac{1}{T_-} - \frac{1}{T_+}\right) \qquad [18]$$

The conjecture that such a relation might be valid in this case has been confirmed by numerical analysis. It is worth stressing that, in this out-of-equilibrium setup, the probability distribution, $P_\tau(z)$, is not Gaussian and exhibits a peculiar asymmetric shape. Nonetheless, for increasing values of τ, the asymmetry progressively reduces, while $P_\tau(z)$ approaches a Gaussian shape. This observation indicates that, in this case, large fluctuations deviate from the typical statistics of independent events.

It should be mentioned that generalized fluctuation–dissipation relations, like those discussed in this section, have been successfully checked in many other situations, where the hypotheses of the Gallavotti–Cohen theorem did not apply. The "robustness" of relations such as [11] and [12] indicates that a more general theory may be possible.

Heat Transport

The validity of Debye's conjecture about the necessity of nonlinear forces for obtaining a finite heat conductivity in crystals still remained an open problem after the unsuccessful FPU numerical experiment. The setup, described in the previous section for testing the generalized fluctuation–dissipation relation in the FPU chain, can be used also for tackling the verification of this conjecture. Actually, the thermal conductivity, κ, of a chain of oscillators can be measured from the Fourier's law

$$J_Q = -\kappa\nabla T(x) \qquad [19]$$

where J_Q is the heat current and $\nabla T(x)$ is the temperature gradient.

This problem was solved analytically for a chain of N harmonic oscillators (Rieder *et al.* 1967). The bulk of the chain is found to reach thermal equilibrium conditions at the average temperature $T = (T_+ + T_-)/2$, corresponding to a constant temperature profile. Only at the chain boundaries the harmonic chain exhibits a steep temperature gradient. This implies that the heat current is proportional to the temperature difference, rather than to the temperature gradient, thus violating Fourier's law. Accordingly, a harmonic chain, made of N oscillators, in contact with two heat reservoirs at different temperatures, exhibits anomalous transport properties and the effective thermal conductivity is found to diverge in the infinite-chain limit as $\kappa \sim N$. This peculiar behavior is a consequence of the integrability of the harmonic chain dynamics. Actually, the Fourier modes propagate with finite velocity through the harmonic chain, so that any energy injected from the hot reservoir flows ballistically to the cold one, rather than diffusing, as required for the validity of [19]. It is worth stressing that any integrable system should exhibit a similar scenario. This is the case of the equal-mass hard sphere gas in one dimension and of the Toda chain, where the harmonic potential $(\omega^2/2)(q_{i+1} - q_i)^2$ is replaced by the nonlinear expression

$$a\exp[-b(q_{i+1} - q_i)]$$

In the former case, integrability and ballistic propagation are straightforward consequences of

the conservation laws, inherent elastic collisions between hard spheres. In the latter model, the normal nonlinear modes, called "Toda solitons," are responsible for such anomalous behavior.

Debye's conjecture should be modified accordingly: nonintegrability of the equations of motion has to be invoked as a necessary property for explaining heat transport in real solids. Let us observe that the FPU model is known not to be integrable and it is expected to be a good candidate for confirming Debye's conjecture, at least in its fully chaotic regime. Careful and extended numerical simulations have shown that the FPU chain maintains anomalous properties (Lepri *et al.* 1997). In particular, the thermal conductivity, κ, is found to diverge in the infinite chain limit as

$$\kappa \sim N^{\gamma} \qquad [20]$$

with $\gamma \approx 2/5$. This value agrees with independent analytic estimates (e.g., see Lepri *et al.* (2003)), although renormalization arguments indicate that one should rather find $\gamma = 1/3$ (Narayan and Ramaswamy 2002). This discrepancy could be due to the peculiar features associated with the presence of a quartic nonlinearity in the FPU problem and also to the fact that in the FPU chain heat can be transported only through longitudinal oscillations. Anyway, this is still an open problem, which requires further theoretical advances to be solved.

In a more general perspective, the main outcome of these numerical studies indicates that a power-law divergence like [20] is found in all one-dimensional nonintegrable models. This general feature must be attributed to the combined effect of low-space dimensionality, with energy and momentum conservation. In such a situation, fluctuations are strongly constrained, so that the evolution of long-wavelength hydrodynamic modes is not sufficiently damped, to be ruled by diffusion (which is a necessary ingredient for the validity of [19]). It must be stressed that these numerical investigations have strongly revived the interest for this problem. In particular, they have also stimulated new theoretical efforts for explaining the power-law divergence of transport coefficients in $d = 1$. One of the main achievements of these theoretical approaches is that the power-law divergence turns to a logarithmic one in $d = 2$, while the divergence should disappear in $d \geq 3$. Despite the difficulty of performing the necessary large-scale simulations for such systems in $d > 1$, it seems that numerics essentially agree with such predictions.

One can find normal transport properties even in $d = 1$, if suitable models are considered. For instance, momentum conservation can be broken by adding to the Hamiltonian [1] a local interaction potential, $U(q_i)$, which breaks translation invariance, thus restoring finite heat conductivity (e.g., see Casati *et al.* 1984). The exception to this case is the harmonic chain with the addition of a local harmonic potential: in this case the dynamics is still integrable and there are as many conserved quantities as degrees of freedom. A further peculiar case is represented by the rotator model in $d = 1$, which is known to be nonintegrable. Its Hamiltonian contains the interaction potential $\epsilon[1 - \cos(q_{i+1} - q_i)]$, replacing the algebraic potentials of the FPU chain. Anyway, such a Hamiltonian still guarantees momentum conservation, since the nearest-neighbor form of the interaction is maintained. Notice that, for small oscillations around the equilibrium position, also the rotator potential admits a Taylor-series expansion, whose first three terms correspond to quadratic, cubic, and quartic contributions, as in the FPU chain. Nonetheless, at variance with the FPU problem, the potential of the rotator model is bounded also from above. Numerical investigations (Giardina *et al.* 2000) have shown that for any finite energy density and for a sufficiently long finite time, some previously oscillating rotators start to rotate, due to local energy fluctuations, that allow to overtake the potential barrier. These dynamical configurations typically appear in the form of spatially localized, synchronous rotating clusters. Their time evolution is characterized by an intermittent behavior: they are eventually reabsorbed by lattice fluctuations and may reappear afterwards at other lattice positions. In this way they play the role of scattering centers for hydrodynamic modes. It must be pointed out that such a qualitative argument is not sufficient for explaining the onset of a genuine diffusive behavior, compatible with the validity of Fourier's law. A hydrodynamic theory, still to be developed, could provide a more convincing insight on these results.

It is worth concluding this section by mentioning that the overall scenario described above is confirmed by numerical studies, relying upon a different approach, based on equilibrium measurements. Actually, the linear response theory by Green and Kubo (see Kubo (1985)) provides an alternative, but essentially equivalent, definition of the thermal conductivity, according to the expression

$$\kappa = \frac{1}{K_B T^2} \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{N} \int_0^t \mathrm{d}\tau \langle J(\tau) J(0) \rangle \qquad [21]$$

The crucial quantity to be computed numerically is the heat-flux time-correlation function $C_J(\tau) = \langle J(\tau)J(0)\rangle$, where $\langle\ \rangle$ represents the thermodynamic equilibrium average. In practice, numerical simulations can be performed for a chain of N oscillators in contact with boundary heat reservoirs at the same temperature $T = T_+ = T_-$. The presence of anomalous transport coefficients can be singled out by analyzing the long-time behavior of $C_J(\tau)$. It has to decay at least as $\tau^{-(1+\varepsilon)}$, with $\varepsilon > 0$ to yield a finite heat conductivity. In one-dimensional models exhibiting the power-law divergence [20] one rather finds

$$C_J(\tau) \sim \tau^{-1+\gamma} \qquad [22]$$

where the positive exponent γ is the same appearing in [20]. This relation between space and time exponents can be easily explained, by considering that space and time variables depend linearly on each other through a proportionality constant, which is the velocity of sound in the lattice. Since $0 < \gamma < 1$, the anomalous behavior observed in out-of-equilibrium conditions is recovered.

One major problem in performing proper numerical studies concerns the control over finite-size effects, which demands a consistent increase of the integration time with the system size. This may yield very extended and expensive computations, mainly when very slow relaxation processes set in. This is the case of the low-energy regime originally studied by FPU in their pioneering computer simulations. Numerical analysis indicates that in this regime the expected behavior of $C_J(\tau)$, reported in eqn [22], sets in after a crossover time t_c, which increases, for decreasing energy density ϵ, as $t_c \approx \epsilon^{-2}$. This seems to be compatible with the studies described earlier.

We conclude this section by pointing out that this result also contributes significantly to clarify one of the basic questions raised by the FPU numerical experiment.

See also: Dynamical Systems and Thermodynamics; Ergodic Theory; Fourier Law; Gravitational *N*-Body Problem (Classical); Lyapunov Exponents and Strange Attractors; Nonequilibrium Statistical Mechanics: Dynamical Systems Approach.

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Nonlinear Schrödinger Equations

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Historical Background

Ginzburg–Landau Equations

Nonlinear Schrödinger (NLS) equations have become one of the most important nonlinear systems studied in mathematics and physics. Actually, one can find the essence of NLS equations in the early work of Ginzburg and Landau (1950) and Ginzburg (1956) in their study of the macroscopic theory of superconductivity, and also of Ginzburg and Pitaevskii (1958), who subsequently investigated the theory of superfluidity.

By minimizing the free energy of a superconductor near the superconducting transition, Ginzburg and Landau arrived at what are now called the Ginzburg–Landau equations:

$$\frac{1}{2m}\left(-\mathrm{i}\hbar\nabla - \frac{e}{c}A\right)^2\psi + \alpha\psi + \beta|\psi|^2\psi = 0 \qquad [1]$$

$$J = -\frac{\mathrm{i}e\hbar}{mc}[\psi^*\nabla\psi - \psi\nabla\psi^*] - \frac{e^2}{mc}|\psi|^2 A \qquad [2]$$

where α, β are phenomenological parameters, A the electromagnetic vector potential, and ψ^* denotes complex conjugate of ψ. The first equation determines the field ψ based on the applied magnetic field. The second equation provides the superconducting current J.

The equation describing the behavior of superfluid helium near the transition point in the stationary case derived in Ginzburg and Pitaevskii (1958) is completely analogous to eqn [1] in the phenomenological theory of superconductivity.

Equation [1] contains all the ingredients of the NLS equations which are discussed below. However, it was not until the 1960s that the wide physical importance of NLS equation became evident. The next section discusses how the NLS equation historically first appeared in the context of nonlinear optics.

Nonlinear Optics: Self-Focusing of Optical Beams in Nonlinear Media

In the mid-1960s, Chiao *et al.* (1964) and Talanov (1964) investigated the conditions under which an electromagnetic beam can produce its own dielectric waveguide and propagate without spreading. This is a reflection of the phenomenon of self-focusing. In fact, self-focusing of optical beams may occur in materials whose dielectric constant increases with field intensity. In the general situation, a beam of uniform intensity in a dielectric broadens due to diffraction. However, the refractive index of many physically important materials (the so-called Kerr materials, such as silica) depends on the field intensity as follows:

$$n = n_0 + n_2|E|^2 + \cdots$$

If the term $n_2|E|^2$ is large enough, the critical angle for total internal reflection at the beam's boundary can be greater than the angular divergence due to diffraction; thus, spreading does not occur as a result of diffraction. As a consequence, a beam above a certain critical power level is trapped and does not spread.

In a remarkable contribution, Kelley (1965) observed, using computational methods (years before computational methods became easy to implement and, consequently, so popular) that when the self-focusing effect due to the increase in the nonlinear index is not compensated by diffraction, there is a buildup in intensity of part of the beam as a function of the distance in the direction of propagation. Consequently, the intensity of the self-focused regions tended to become "anomalously large," that is, a singularity appeared to develop.

Consider as starting equation the electromagnetic wave equation in the presence of nonlinearities derived earlier by Chiao *et al.* (1964):

$$\nabla^2 E - \frac{\epsilon_0}{c^2}\partial_t^2\, E - \frac{\epsilon_2}{c^2}\partial_t^2\, (E^2 E) = 0 \qquad [3]$$

where $\epsilon_2|E|^2 \ll 1$. One assumes a linearly polarized wave of frequency ω, propagating along the z-axis, so that

$$E = \tfrac{1}{2}(\mathcal{E}\mathrm{e}^{\mathrm{i}(kz-\omega t)} + \mathrm{c.c.})\hat{e}$$

where c.c. denotes complex conjugation, $k = \epsilon_0^{1/2}\omega/c$, the factor $\exp(\mathrm{i}kz - \omega t)$ represents the propagating part, that is, the "carrier," of the wave, and $\mathcal{E}$ is the slowly varying part. Substituting the above expression for E into eqn [3], neglecting the third-harmonic term and the term $\partial_z^2\mathcal{E}$ from $\nabla^2 E$ (assuming it to be small), yields

$$2\mathrm{i}k\partial_z\mathcal{E} + \left(\partial_x^2 + \partial_y^2\right)\mathcal{E} + \frac{3}{4}k^2\frac{\epsilon_2}{\epsilon_0}|\mathcal{E}|^2\mathcal{E} = 0 \qquad [4]$$

or, with a suitable rescaling of the dependent and independent variables ($\mathcal{E} \to \psi/((3/4)k^2\epsilon_2/\epsilon_0)^{1/2}$, $z \to 2kz$),

$$i\partial_z\psi + \nabla_\perp^2\psi + 2|\psi|^2\psi = 0 \qquad [5]$$

which is the NLS equation in standard nondimensional form.

It should be remarked here that the name NLS equation for equations of the form of [5] is natural due to the formal analogy with the Schrödinger equation in quantum mechanics:

$$i\partial_t\psi + \nabla^2\psi + V\psi = 0 \qquad [6]$$

If one sets $V = 2|\psi|^2$ in eqn [6], the result is the NLS equation. In the context of quantum mechanics, a nonlinear potential arises in the "mean-field" description of interacting particles.

Modifications of [6] also arise as mean-field descriptions of Bose–Einstein condensates which is of keen interest in physics (see Pethick and Smith (2002) and references therein). The normalized equation is

$$i\partial_t\psi - \nabla^2\psi + \left(V(x,y) + 2|\psi|^2\right)\psi = 0 \qquad [7]$$

where V is an external potential. This is generally referred to as the Gross–Pitaevskii equation.

Talanov (1965) (see also Zakharov *et al.* (1971)) investigated the behavior of stationary light beams in a self-focusing nonlinear medium and found that for a purely cubic nonlinearity, "collapse" of the beam can take place. The proof that there is a singularity in eqn [5] is remarkably straightforward. This is discussed in the section "Wave collapse." In order to avoid wave collapse, other physical effects (e.g., saturable nonlinearity or dissipation) are required.

Universal Character of the NLS Equation

It turns out that almost any dispersive, energy-preserving system gives rise, in an appropriate limit, to the NLS equation. For instance, one can derive the NLS from other physically significant equations such as the Klein–Gordon equation

$$u_{tt} - u_{xx} + u + ku^3 = 0$$

and the Korteweg–de Vries (KdV) equation

$$u_t + 6uu_x + u_{xxx} = 0$$

Actually, the NLS equation provides a "canonical" description for the envelope dynamics of a quasi-monochromatic plane wave (the carrier wave) propagating in a weakly nonlinear dispersive medium when dissipative processes are negligible.

Indeed, consider a scalar nonlinear wave equation written symbolically as

$$L(\partial_t, \nabla)u + G(u) = 0$$

where L is a linear differential operator with constant coefficients and G a nonlinear function of u and its derivatives. For a real, small-amplitude solution of magnitude $\epsilon \ll 1$, the nonlinear effects can first be neglected, and the equation admits approximate monochromatic wave solutions

$$u = \epsilon\psi e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega t)} + \text{c.c.} \qquad [8]$$

with small amplitude $\epsilon|\psi|$. Substituting [8] into the linear equation, one can find that the frequency ω and the wave vector $\boldsymbol{k}$ are related by the dispersion relation

$$L(-i\omega, i\boldsymbol{k}) = 0$$

Let

$$\omega = \omega(\boldsymbol{k})$$

be one of the solutions of the previous equation. Suppose one is interested in a solution ψ which is not constant, but slowly varying in space and time. This has the interpretation of $\boldsymbol{k}$ having a "sideband" wave vector and ω a "sideband" frequency. More precisely, restricting discussion, for simplicity, to the $(1+1)$-dimensional case, the slowly varying amplitude assumption corresponds to letting

$$\psi(x,t) = \psi(X,T) = \psi_0 e^{i(Kx - \Omega t)}$$

where $X = \epsilon x$ and $T = \epsilon t$. Note that $K = \epsilon k$ and $\Omega = \epsilon\omega$ are sometimes referred to as the sideband wave number and frequency, respectively, because they correspond to a deviation from the central wave number k and central frequency ω. Looking at these deviations from the point of view of operators, whereby $\omega \to i\partial_t$, $k \to -i\partial_x$ and $\Omega \to i\partial_T$, $K \to -i\partial_X$, one has

$$\omega_{\text{tot}} \sim \omega + \epsilon\Omega = \omega + i\epsilon\partial_T$$
$$k_{\text{tot}} \sim k + \epsilon K = k - i\epsilon\partial_X$$

Then $\omega(k)$ can be expanded in a Taylor series around the central wave number as

$$\omega(k - i\epsilon\partial_X) \sim \omega(k) - i\epsilon\omega'\partial_X - \epsilon^2\frac{\omega''}{2}\partial_X^2 + \cdots$$

Therefore,

$$\omega_{\text{tot}}(k)\psi \sim [\omega(k) + i\epsilon\partial_T]\psi$$
$$\sim \left(\omega(k) - i\epsilon\omega'\partial_X - \epsilon^2\frac{\omega''}{2}\partial_X^2\right)\psi$$

which shows that, to the leading order,

$$\mathrm{i}\epsilon\left(\frac{\partial\psi}{\partial T}+\omega'\frac{\partial\psi}{\partial X}\right)+\epsilon^2\frac{\omega''}{2}\frac{\partial^2\psi}{\partial X^2}=0 \qquad [9]$$

In the moving frame $\xi = X - \omega'(k)T$, $\tau = \epsilon T \equiv \epsilon^2 t$, eqn [9] transforms to

$$\epsilon^2\left(\mathrm{i}\psi_\tau+\frac{\omega''}{2}\psi_{\xi\xi}\right)=0$$

which is the linear Schrödinger equation with the canonical $\omega''(k)/2$ coefficient. On the other hand, if one considers rather general conservative nonlinear wave problems with leading quadratic or cubic nonlinearity, asymptotic analysis (e.g., multiple scale analysis which yields the so-called Stokes–Poincaré frequency shift) shows that a wave solution of the form

$$u(x,t)=\epsilon\psi(\tau)\mathrm{e}^{\mathrm{i}(kx-\omega t)}+\mathrm{c.c.}$$

with $\tau = \epsilon^2 t$ has $\psi(\tau)$ satisfying

$$\mathrm{i}\frac{\partial\psi}{\partial\tau}+n|\psi|^2\psi=0 \qquad [10]$$

where the constant coefficient n depends on the particular equation under study. It should be remarked here that cubic nonlinearity yields an $O(\epsilon^3)$ contribution, which is balanced by a slow timescale of order ϵ^2. Putting the linear and nonlinear effects together (i.e., eqns [9] and [10]) implies that an NLS equation of the form

$$\mathrm{i}\frac{\partial\psi}{\partial t}+\frac{\omega''}{2}\frac{\partial^2\psi}{\partial\xi^2}+n|\psi|^2\psi=0$$

naturally arises. The NLS equation is viewed as a "universal" equation as it generically governs the slowly varying envelope of a monochromatic wave train (see also Benney and Newell (1969)).

Physical Applications

The nonlinear propagation of wave packets is governed by NLS-type systems in several different branches of scientific and technological applications, beyond what has been mentioned earlier. Some of these applications are discussed below.

NLS equation in Water Waves

The NLS equation in the context of small-amplitude water waves was derived by Zakharov (1968) (infinite depth) and Benney and Roskes (1969) (finite depth). The procedure for deriving the NLS equation from the Euler–Bernoulli equations of fluid dynamics in one horizontal direction will now be discussed, under the assumption of small-amplitude waves and deep water. The interested reader can also find the details of the derivation in Ablowitz and Clarkson (2006). The relevant equations are

$$\phi_{xx}+\phi_{zz}=0, \quad -\infty<z<\epsilon\eta(x,t) \qquad [11]$$

$$\phi_z=0, \quad z\to-\infty \qquad [12]$$

$$\phi_t+\frac{\epsilon}{2}(\phi_x^2+\phi_z^2)+g\eta=0, \quad z=\epsilon\eta \qquad [13]$$

$$\eta_t+\epsilon\eta_x\phi_x=\phi_z, \quad z=\epsilon\eta \qquad [14]$$

where ϕ is the velocity potential of an ideal (i.e., incompressible, irrotational, and inviscid) fluid, $\eta(x,t)$ is the free surface of the fluid, which is to be found, in addition to $\phi(x,z;t)$.

Equation [11] expresses the ideal nature of the fluid; the condition [12] expresses the requirement that there is no vertical flow at infinity; and eqn [13] is the Bernoulli equation of energy conservation. Finally, eqn [14] is a kinematic condition stating that no flow occurs transverse to the free surface.

At the free boundary, for small amplitudes, one can expand $\phi = \phi(t,x,\epsilon\eta)$ for $\epsilon \ll 1$ as

$$\phi=\phi(t,x,0)+\epsilon\eta\phi_z(t,x,0)+\frac{(\epsilon\eta)^2}{2}\phi_{zz}(t,x,0)+\cdots$$

and similarly for the derivatives. Second, one introduces slow temporal and spatial scales (one expects the slowly varying envelope of the wave to depend on slow variables $X = \epsilon x$, $Z = \epsilon z$, $T = \epsilon t$). Finally, because of the quadratic nonlinearity one expects second harmonics to be generated; hence,

$$\phi=\left(A\mathrm{e}^{\mathrm{i}\Theta+|k|z}+\mathrm{c.c.}\right)+\epsilon\left(A_2\mathrm{e}^{2\mathrm{i}\Theta+2|k|z}+\mathrm{c.c.}+\bar{\phi}\right)$$

$$\eta=\left(B\mathrm{e}^{\mathrm{i}\Theta}+\mathrm{c.c.}\right)+\epsilon\left(B_2\mathrm{e}^{2\mathrm{i}\Theta}+\mathrm{c.c.}+\bar{\eta}\right)$$

where A, A_2, $\bar{\phi}$ depend on X, Z, T and B, B_2, $\bar{\eta}$ depend on X, T ($\bar{\phi}$ and $\bar{\eta}$ are mean contributions, which are real) and $\Theta = kx - \omega t$ with the dispersion relation $\omega^2 = g|k|$. Substituting this ansatz into the equations, one obtains from the order-ϵ^2 terms

$$2\mathrm{i}\omega A_\tau-\left(\frac{v_{\mathrm{g}}^2}{2\omega}A_{\xi\xi}+\frac{2k^4}{\omega}|A|^2A\right)=0 \qquad [15]$$

where $v_{\mathrm{g}} = \omega'(k) = g/2\omega$ is the group velocity and the new variables $\tau = \epsilon T$, $\xi = X - v_{\mathrm{g}}T$.

Equation [15] is the typical formulation of the (1 + 1)-dimensional NLS equation found in water wave theory for large depth.

In the section "NLS in nonlinear optics," a special solution to (a rescaled version of) eqn [15], namely a soliton solution, is discussed in the

context of nonlinear optics. It should be remarked here that the coefficients of both terms $A_{\xi\xi}$ and $|A|^2A$ have the same sign. This is necessary for a decaying soliton solution to exist (see, e.g., Lighthill (1965)).

NLS in Nonlinear Optics

The NLS equation also describes self-compression and self-modulation of electromagnetic wave packets in weakly nonlinear media. Hasegawa and Tappert (1973a, b) first derived the NLS equation in the context of fiber optics. Light-wave propagation in a fiber is mainly affected by: (1) group velocity dispersion (GVD), that is, the frequency dependence of the group velocity originating from the refractive index of the fiber and (2) fiber nonlinearity (the so-called Kerr effect), originating from the dependence of the refractive index on the intensity of the optical pulse. In the presence of GVD and Kerr nonlinearity, the refractive index is expressed as

$$n(\omega, E) = n_0(\omega) + n_2|E|^2 \qquad [16]$$

where ω and E represent the frequency and electric field of the light wave, respectively, $n_0(\omega)$ is the frequency-dependent linear refractive index, and the constant n_2, referred to as the Kerr coefficient, is "small" but can have significant impact since the nonlinear effects accumulate over long distances. Normally, the electric field is modulated into a slowly varying amplitude of a carrier wave:

$$E(z,t) = \mathcal{E}(z,t)e^{i(k_0z-\omega_0t)} + \text{c.c.} \qquad [17]$$

where z denotes the distance along the fiber, t the time, $k_0 = k_0(\omega_0)$ the wave number, ω_0 the frequency, and $\mathcal{E}(z,t)$ the envelope of the electromagnetic field.

A Taylor series expansion of the dispersion relation (see also the section "Universal character of the NLS equation")

$$k(\omega, E) = \frac{\omega}{c}(n_0(\omega) + n_2|E|^2)$$

around the carrier frequency $\omega = \omega_0$ yields

$$k - k_0 = k'(\omega_0)(\omega - \omega_0) + \frac{k''(\omega_0)}{2}(\omega - \omega_0)^2 + \frac{\omega_0 n_2}{c}|E|^2 \qquad [18]$$

where the prime represents derivative with respect to ω and $k_0 = k(\omega_0)$. Replacing $k - k_0$ and $\omega - \omega_0$ by their Fourier operator equivalents, $i\partial_z$ and $i\partial_t$ resp., using $k - k_0 = (\omega/c)n_0(\omega)$ and letting eqn [18] operate on $\mathcal{E}$ yields

$$i\left(\frac{\partial\mathcal{E}}{\partial z} + k_0'(\omega_0)\frac{\partial\mathcal{E}}{\partial t}\right) - \frac{k_0''(\omega_0)}{2}\frac{\partial^2\mathcal{E}}{\partial t^2} + \nu|\mathcal{E}|^2\mathcal{E} = 0 \quad [19]$$

where $\nu = \omega_0 n_2/cA_{\text{eff}}$, with A_{eff} being the effective cross-section area of the fiber (the factor $1/A_{\text{eff}}$ comes from a more detailed derivation which takes into account the finite size of the fiber; the factor $1/A_{\text{eff}}$ is needed in order to account for the variation of field intensity in the cross section of the fiber). Note that $k_0'(\omega_0) = 1/v_g$, where v_g represents the group velocity of the wave train. Introducing dimensionless variables $t' = t_{\text{ret}}/t_*, z' = z/z_*, q = \mathcal{E}/\sqrt{P_*}$ yields the NLS equation

$$i\frac{\partial q}{\partial z'} + \frac{\text{sgn}(-k_0''(\omega_0))}{2}\frac{\partial^2 q}{\partial t'^2} + |q|^2q = 0 \qquad [20]$$

where t_*, P_* are the characteristic time and power, respectively, and $t_{\text{ret}} = t - k_0'(\omega_0)z = t - z/v_g$, $z_* = 1/\nu P_*$, with the constraint that the "nonlinear length" is balanced by the linear dispersion time, that is, $t_* = (z_*| - k''(\omega_0)|)^{1/2}$.

There are two cases of physical interest depending on the sign of k_0''. The so-called focusing case occurs when $k_0'' < 0$; this is called "anomalous" dispersion. The defocusing case obtains when the dispersion is "normal": $k_0'' > 0$.

Now write eqn [20] in the form

$$iq_t + q_{xx} \pm 2|q|^2q = 0 \qquad [21]$$

with $\pm$ corresponding to the focusing (+) and defocusing (–) case, respectively. The focusing NLS equation admits special solutions called "bright" solitons (solutions that are traveling localized "humps"). A pure one-soliton solution in the focusing (+) case has the form

$$q(x,t) = \eta\,\text{sech}[\eta(x + 2\xi t - x_0)]\,e^{-i\Theta} \qquad [22]$$

where $\Theta = \xi x + (\xi^2 - \eta^2)t + \Theta_0$. The parameters ξ and η are such that $\lambda = \xi/2 + i\eta/2$ is an eigenvalue from the inverse scattering transform analysis.

The defocusing (–) NLS equation does not admit solitons that decay at infinity. However, it does admit soliton solutions which have a nontrivial background intensity (called "dark" and "gray" solitons). A dark-soliton solution has the form

$$q(x,t) = \eta\,\tanh(\eta x)\,e^{-2i\eta^2 t} \qquad [23]$$

Note that $q \to \pm\eta$ as $x \to \pm\infty$. A gray-soliton solution is

$$q(x,t) = \eta\left[1 - B^2\,\text{sech}^2(\eta B(x - x_0))\right]^{1/2} e^{i\phi(x,t)} \quad [24]$$

with

$$\phi(x,t) = -\eta^2(2-B^2)t + \eta\sqrt{1-B^2}x + \tan^{-1}\left(\frac{B\tanh(\eta Bx)}{\sqrt{1-B^2}}\right) + \phi_0$$

and $|B| < 1$. Note that as $B \to 1^-$, the gray soliton becomes a dark soliton, taking $\phi_0 = -\pi/2$.

Recall that the solutions [23] and [24] can be allowed to travel uniformly by making a Galilean transformation, that is, taking into account that if $q_1(x,t)$ is a solution of [21], then so is

$$q_2(x,t) = q_1(x - vt, t)\,e^{i(kx-\omega t)}$$

with $k = -v$ and $\omega = -k^2/2$.

It should also be remarked that Ablowitz *et al.* (1997) have shown that, in quadratically nonlinear optical materials, more complicated NLS-type equations arise. These equations are analogous to the finite-depth multidimensional nonlocal NLS-type systems derived in the context of water waves by Benney and Roskes (1967) and later by Davey and Stewartson (1974).

Optical Communications

Hasegawa and Tappert (1973) first suggested using solitons as the "bit" format for transmission of information in optical fiber systems. Motivated by this, in 1980, scientists at Bell Laboratories observed solitons (described by the NLS equation) in optical fibers (Mollenauer *et al.* 1980). The development of optical amplifiers (erbium-doped amplifiers) in the mid-1980s provided a mechanism to compensate fiber loss, and this permitted the transmission of information entirely optically over long distances. With damping and amplification included (see, e.g., Hasegawa and Kodama (1995)), the NLS equation [20] takes the form

$$i\frac{\partial q}{\partial z} + \frac{\mathrm{sgn}(-k_0''(\omega_0))}{2}\frac{\partial^2 q}{\partial t^2} + g(z)|q|^2 q = 0 \qquad [25]$$

where $g(z) = a_0^2 \exp(-2\Gamma z/z_a), 0 < z < z_a$, and periodically extended thereafter, and a_0^2 is determined by

$$< g > = \frac{1}{z_a}\int_0^{z_a} g(z/z_a)\mathrm{d}z = 1$$

with $z_a = l_a/z_*, l_a$ being the amplifier length. Remarkably, asymptotic analysis ($z_a \ll 1$) shows that, to leading order, $q(z,t)$ still satisfies the NLS equation [20].

Amplifiers, however, introduce small amounts of noise to the system, which causes the temporal position of the soliton to fluctuate (cf. Gordon and Haus (1986)) and thus limits the distance signals can be reliably transmitted to. Soliton control mechanisms were introduced in the early 1990s in order to deal with these difficulties (cf. Mecozzi *et al.* (1991) and Kodama and Hasegawa (1992)).

By the mid-1990s, the development of all optical transmission systems began to take great advantage of wavelength-division-multiplexing (WDM), that is, the simultaneous transmission of multiple signals in different frequency (or equivalently wavelength) "channels" (Hasegawa 2000). However, it was found that a serious problem affected WDM systems. Namely, the interactions of solitons traveling at different velocities cause resonant amplifier-induced instabilities in adjacent frequency channels (four-wave mixing (Mamyshev and Mollenauer 1996, Ablowitz *et al.* 1996)). In order to avoid these instabilities, researchers developed and analyzed dispersion-managed (DM) transmission systems (cf. Hasegawa (2000)). In a DM transmission system, the fiber is composed of alternating sections of positive (normal) and negative (anomalous) dispersion fibers. The (dimensionless) NLS equation that governs this phenomenon is

$$i\frac{\partial q}{\partial z} + \frac{d(z)}{2}\frac{\partial^2 q}{\partial t^2} + g(z)|q|^2 q = 0 \qquad [26]$$

where $d(z)$ is usually taken to be a periodic, large, rapidly varying function of the form $d(z) = \delta_a + \Delta(z)$, with $|\Delta(z)| \gg 1$ and having zero average in the period z_a (generally the same as that of the amplifier). In fact, asymptotic analysis of [26] yields a nonlocal NLS-type equation (Gabitov and Turitsyn 1996, Ablowitz and Biondini 1998). It has also been shown that eqn [26] admits various types of optical pulses, such as DM solitons (Ablowitz and Biondini 1998), and quasilinear modes (Ablowitz *et al.* 2001).

NLS Equation in Other Settings

Many other interesting applications of the NLS equations exist in such different areas of physics as magnetic spin waves (see, e.g., the work by Zvezdin and Popkov (1983) and also by Kalinikos *et al.* (1997)), plasma physics (cf. the work by Zakharov (1972) on collapse of Langmuir waves), other areas of fluid dynamics, etc. (the interested reader can find an overview in the monograph by Ablowitz (1981)).

Mathematical Framework

Mathematically, the NLS equation had attained broad significance since it is integrable via

inverse-scattering transform (IST), admits multisoliton solutions, has an infinite number of conserved quantities, and possesses many other interesting properties. Some of these are discussed below.

The Inverse-Scattering Transform

The IST method allows one to linearize a large class of nonlinear evolution equations and can be considered as a nonlinear version of the Fourier transform. An essential prerequisite of IST method is the association of the nonlinear evolution equation with a pair of linear problems (Lax pair), a linear eigenvalue problem, and a second associated linear problem, such that the given equation results as a compatibility condition between them. A key research breakthrough on NLS systems appeared in 1972, in the papers of Zakharov and Shabat (1972, 1973), who first analyzed the scalar NLS equation in the form

$$\mathrm{i}q_t = q_{xx} \pm 2|q|^2 q \qquad [27]$$

($\pm$ correspond to the focusing/defocusing case, respectively) and found the associated Lax pair

$$v_x = \begin{pmatrix} -\mathrm{i}k & q \\ \mp q^* & \mathrm{i}k \end{pmatrix} v \qquad [28]$$

$$v_t = \begin{pmatrix} 2\mathrm{i}k^2 \mp \mathrm{i}|q|^2 & -2kq - \mathrm{i}q_x \\ \pm 2kq^* \mp \mathrm{i}q_x^* & -2\mathrm{i}k^2 \pm \mathrm{i}|q|^2 \end{pmatrix} v \qquad [29]$$

where $v(x,t)$ is a two-component vector. The compatibility of [28] and [29] yields eqn [27], assuming that the eigenvalue parameter k is constant in time (so that [27] is often said to be isospectral).

The solution of the initial-value problem of a nonlinear evolution equation by IST proceeds in three steps, as follows:

1. *the forward problem* – the transformation of the initial data from the original "physical" variables to the transformed "scattering" variables;
2. *time dependence* – the evolution of the transformed data according to simple, explicitly solvable evolution equations; and
3. *the inverse problem* – the recovery of the evolved solution in the original variables from the evolved solution in the transformed variables.

The implementation of steps 1–3 described above is more concretely carried out as follows. The initial (Cauchy) datum $q(x,0)$ for eqn [27] is mapped into scattering data $S(k,0)$ (comprising, in general, discrete eigenvalues and associated normalization constants, and reflection coefficients) by means of eqn [28]. The data $S(k,0)$ are evolved via eqn [29] to get $S(k,t)$ at an arbitrary time $t > 0$. Finally, by employing the methods of inverse scattering, eqn [28] allows one to reconstruct the evolved solution $q(x,t)$ from $S(k,t)$.

One can easily note the "formal" resemblance to the well-known method of Fourier transform for linear differential equations.

There is considerable literature on the subject and the interested reader is encouraged to consult, for instance, some of the following references: Ablowitz and Segur (1981), Calogero and Degasperis (1982), Novikov *et al.* (1984), Ablowitz and Clarkson (1991), Ablowitz *et al.* (2004).

Linear Stability Analysis

Consider a special solution of eqn [27] in the focusing (+sign) case: $q = a\exp(-2\mathrm{i}a^2 t)$. If this solution is perturbed as

$$q(x,t) = a\mathrm{e}^{2\mathrm{i}a^2 t}(1 + \epsilon(x,t))$$

where $|\epsilon| \ll 1$, it is found that ϵ satisfies the condition

$$\mathrm{i}\epsilon_t = \epsilon_{xx} + 2a^2(\epsilon + \epsilon^*)$$

On the periodic spatial domain $0 < x < L$, ϵ has the Fourier expansion

$$\epsilon(x,t) = \sum_{-\infty}^{\infty} \hat{\epsilon}_n(t)\mathrm{e}^{\mathrm{i}\mu_n x}$$

where

$$\mu_n = \frac{2\pi n}{L} \qquad [30]$$

Assuming a solution of the form

$$\begin{pmatrix} \hat{\epsilon}_n \\ \hat{\epsilon}_{-n}^* \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \mathrm{e}^{\mathrm{i}\sigma_n t}$$

one finds that σ_n satisfies

$$\sigma_n^2 = \mu_n^2(\mu_n^2 - 4a^2) \qquad [31]$$

It then turns out that when $aL/\pi < n$ the system is unstable. Note that there are only a finite number of unstable modes (i.e., for fixed a, L, sufficiently high mode numbers n will not satisfy the above inequality). In the context of water waves, this corresponds to the famous experimental and theoretical result by Benjamin and Feir that the Stoke's water wave is unstable. Later, Benney and Roskes (1969) showed that all periodic wave solutions of the generalized nonlocal NLS equation resulting from water waves in $(2+1)$-dimensions are unstable. Also, in $(2+1)$-dimensions soliton solutions are unstable to weak transverse modulations.

Wave Collapse

The equation

$$i\psi_t + \Delta\psi + |\psi|^2\psi = 0, \qquad \boldsymbol{x} \equiv (x, y) \in \mathbb{R}^2 \qquad [32]$$

has the following conserved quantities:

$$P = \int |\psi|^2 \, d\boldsymbol{x}$$

$$\boldsymbol{M} = \int \psi \nabla \psi \, d\boldsymbol{x}$$

$$H = \int \left[|\nabla\psi|^2 - \frac{1}{2}|\psi|^4 \right] d\boldsymbol{x}$$

that is, mass (power), momentum, and energy (Hamiltonian) are conserved. Remarkably, Talanov (1965) showed that eqn [32] satisfies the following equation:

$$\frac{\partial^2 V}{\partial t^2} = 8H \qquad [33]$$

where

$$V = \int (x^2 + y^2)|\psi|^2 \, dx \, dy$$

Equation [33] is also known as the "virial" theorem. Hence, it follows that

$$V = 4Ht^2 + c_1 t + c_2$$

and if $H < 0$ initially, then a singularity in eqn [32] results since V must be positive. Actually, one can further show (see, e.g., C Sulem and P L Sulem (1999), and references therein) that there exists a time t^* such that

$$\int |\nabla\psi|^2 \, d\boldsymbol{x}$$

becomes infinite as $t \to t^*$, which in turn implies that ψ also becomes infinite as $t \to t^*$ (blowup in finite time).

Note also that for the more general equation

$$i\psi_t + \Delta_d\psi + |\psi|^{2\sigma}\psi = 0, \qquad \boldsymbol{x} \in \mathbb{R}^d$$

where Δ_d is the d-dimensional Laplacian, one has the following types of solutions:

- *Supercritical* ($\sigma d > 2$): the solution blows up.
- *Critical* ($\sigma d = 2$): blowup can occur or global solution can exist.
- *Subcritical* ($\sigma d < 2$): global solutions exist.

Vector NLS Systems

In many applications vector NLS (VNLS) systems are the key governing equations. Physically, the VNLS arise under conditions similar to those described by NLS with the additional proviso that there are multiple wave trains moving nearly with the same group velocities (Roskes 1976). Importantly, VNLS also models systems where the field has more than one component. For example, in optical fibers and waveguides, the propagating electric field has two components transverse to the direction of propagation. The nondimensional system

$$iq_z^{(1)} = q_{xx}^{(1)} + 2\left(|q^{(1)}|^2 + |q^{(2)}|^2\right)q^{(1)} \qquad [34a]$$

$$iq_z^{(2)} = q_{xx}^{(2)} + 2\left(|q^{(1)}|^2 + |q^{(2)}|^2\right)q^{(2)} \qquad [34b]$$

is an asymptotic model which governs the propagation of the electric field in a waveguide, where z is the normalized distance along the waveguide and x a transversal spatial coordinate. It was first examined by Manakov (1974) (see also Anastassiou *et al.* (1999) and Soljačić *et al.* (2003)). Subsequently, this system was derived as a key model for light-wave propagation in optical fibers. More precisely, in optical fibers with constant birefringence (i.e., constant phase and group velocities as a function of distance) Menyuk (1987) has shown that the two polarization components of the electromagnetic field $\mathcal{E} = (u, v)^{\mathrm{T}}$ which are orthogonal to the direction of propagation, z, along the fiber asymptotically satisfy the following nondimensional equations (assuming anomalous dispersion):

$$i(u_z + \delta u_t) + \tfrac{1}{2}u_{tt} + (|u|^2 + \alpha|v|^2)u = 0 \qquad [35a]$$

$$i(v_z - \delta v_t) + \tfrac{1}{2}v_{tt} + (\alpha|u|^2 + |v|^2)u = 0 \qquad [35b]$$

where δ represents the group velocity "mismatch" between the u, v components of the electromagnetic field, α is a constant that depends on the polarization properties of the fiber, z the distance along the fiber, and t a retarded temporal frame. In deriving eqn [35], it is assumed that the electromagnetic field is slowly varying (as in the scalar problem); certain nonlinear (four-wave mixing) terms are neglected in the derivation of eqn [35], because the light wave is rapidly varying due to large, but constant, linear birefringence. In this context, birefringence means that the phase and group velocities of the electromagnetic wave in each polarization component are different. In a communications environment, due to the distances involved (hundreds to thousands of kilometers), the polarization properties evolve rapidly and randomly as the light wave evolves along the propagation distance, z. Not only does the birefringence evolve, but it does so randomly, and on a scale much faster than the distances required for

communication transmission (birefringence polarization changes on a scale of 10–100 m). In this case, the relevant nonlinear equation is eqn [35] above, but with $\delta = 0$ and $\alpha = 1$. Indeed, this is the integrable VNLS equation first derived by Manakov (1974).

It should be remarked that the VNLS equation [34] and its generalization to an arbitrary number of components,

$$\mathrm{i}q_t = q_{xx} \pm 2\|q\|^2 q \qquad [36]$$

where q is an N-component vector and $\|\cdot\|$ is the Euclidean norm, are integrable by the IST. One has to suitably extend the analysis discussed earlier in this article (cf. e.g., Ablowitz *et al.* (2004)).

Discrete NLS Systems

Both the NLS and the VNLS equations discussed above admit integrable discretizations which, besides being used as the basis for constructing numerical schemes for the continuous counterparts, also have physical applications as discrete systems.

A natural discretization of NLS [27] is the following:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}q_n = \frac{1}{h^2}(q_{n+1} - 2q_n + q_{n-1}) \pm |q_n|^2(q_{n+1} + q_{n-1}) \qquad [37]$$

which is referred to as the integrable discrete NLS (IDNLS). It is an $O(h^2)$ finite-difference approximation of [27] which is integrable via the IST and has soliton solutions on the infinite lattice (Ablowitz and Ladik 1975, 1976). Note that if the nonlinear term in [37] is changed to $2|q_n|^2 q_n$, the equation, which is often called the discrete NLS (DNLS) equation, is apparently no longer integrable. It should be remarked that the (apparently nonintegrable) DNLS equation arises in many important physical contexts.

Correspondingly, one can consider the discretization of VNLS given by the following system:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}q_n = \frac{1}{h^2}(q_{n+1} - 2q_n + q_{n-1}) \pm \|q_n\|^2(q_{n+1} + q_{n-1}) \qquad [38]$$

where q_n is an N-component vector. Equation [38] for $q_n = q(nh)$ in the limit $h \to 0, nh = x$ gives VNLS [36]. The discrete vector NLS system [38] is also integrable (Ablowitz *et al.* 1999, Tsuchida *et al.* 1999). The interested reader can find further details in Ablowitz *et al.* (2004).

See also: Boundary-Value Problems for Integrable Equations; Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; Evolution Equations: Linear and Nonlinear; Ginzburg–Landau Equation; Integrable Systems and Discrete Geometry; Integrable Systems: Overview; Partial Differential Equations: Some Examples; Riemann–Hilbert Methods in Integrable Systems; Schrödinger Operators.

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Non-Newtonian Fluids

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Introduction

The flow of a fluid, liquid or gas, is described by three conservation laws, the conserved physical quantities being the mass, the linear momentum, and the energy, and by constitutive equations. The constitutive equations are specific to each fluid, and link deformations to stresses.

A fluid is said to be Newtonian if it satisfies the simplest constitutive equation, which gives the stress tensor σ as a linear function of the rate of deformation tensor $\boldsymbol{D} = (1/2)(\nabla u + \nabla u^{\mathrm{T}})$, namely

$$\sigma = (\lambda \operatorname{tr} \boldsymbol{D} - p)\boldsymbol{I} + 2\eta \boldsymbol{D} \qquad [1]$$

where u is the fluid velocity, p is the hydrostatic pressure ($p \geq 0$), and λ and η are the Lamé viscosity coefficients of the fluid, satisfying $\eta \geq 0$ and $\lambda + 2\eta/3 \geq 0$. The superscript T designates the transpose operation, the abbreviation "tr" the trace operator of a tensor, and $\boldsymbol{I}$ the unit tensor. Water and glycerin are examples of Newtonian liquids.

Non-Newtonian fluids are fluids for which the behavior is not described by eqn [1]. Silicone oils, polymers (melted or in solution), egg yolks, and blood are examples of non-Newtonian liquids. Other examples include liquid crystals, rubbers, suspensions, paints, etc.

In the following we shall first describe flows which show Newtonian or non-Newtonian behaviors. Then we shall describe the requirements a constitutive equation needs to satisfy to be considered, introducing the notions of continuum mechanics we need. After giving the most commonly used constitutive equations, we will give a few ideas about the mathematical study of the set of equations, and their numerical study, in the particular case of viscoelastic fluids.

Numerous kinds of materials are already known to exist, and more might exist in the future. This report, however, will be limited to the most commonly materials used nowadays, which are polymers, liquid crystals and polymeric liquids crystals, and paints. Moreover, we shall only consider isothermal flows, even though temperature might be an important parameter in experiments or in industry, because in particular most theoretical or numerical studies concern isothermal problems.

Non-Newtonian fluids will always be liquids, and we shall use the terms liquid or fluid indifferently.

Non-Newtonian Behaviors

We describe a few experiments to show how differently both types of fluids, Newtonian or non-Newtonian, might react in some experimental situations. We also give some mechanical explanation when possible.

Shear Thinning or Shear Thickening

In a Poiseuille experiment, where a fluid flows in a tube under the action of a pressure drop, the volumetric flow rate of a Newtonian fluid is inversely proportional to the constant fluid viscosity. Under the same pressure-drop condition, a polymer melt flows much faster out of the tube, which means that there is a decreasing apparent viscosity with increasing shear rate: this is referred to as shear thinning effect. Other fluids might exhibit the opposite behavior and flow out of the tube more slowly: this is called the shear thickening effect.

Rod Climbing

When a rotating rod is inserted in a beaker filled with a Newtonian fluid, it is observed that the liquid near the rotating rod is pushed outwards by centrifugal force and that a dip on the surface of the liquid near the rod results. On the contrary, if we make the same experiment with a polymer, the fluid climbs along the rod. Moreover, for comparable rotation speed, the difference in behaviors might be quantitatively considerable. This is explained by totally different pressure repartitions in both fluids, Newtonian or non-Newtonian: in particular, the pressure in the polymer along the rod is much larger than that along the beaker, so that this pressure difference fights the centrifugal force; this is in contrast with the situation in a Newtonian fluid.

Extrudate Swell

If a fluid is forced to flow from a large reservoir out of a circular tube of small diameter, the swell at the exit is much larger for a polymer solution than for a Newtonian fluid. A polymer flowing out of a die might also show a delayed die well, which means that the swell is not at the exit but on the jet at a certain distance of the exit. The explanation of this phenomenon is not unique: it is due partly to memory effects (the fluid remembers its former shape, the one in the reservoir), partly to the release of normal stresses, to interfacial forces, compressibility, viscous heating, and the complicated flow near the die exit.

Difference in Normal Stresses

In a shearing flow of a Newtonian fluid, the two normal stress differences are both zero, whereas for a polymer the first normal stress difference might be very large, the second one being nearly zero. These differences in stresses in shearing flow might be a partial answer to the extrudate swell and to rod climbing experienced by polymers.

Presence of a Yield Stress

Some materials, when subjected to shear stress, flow only after a critical value is attained. Such fluids are referred to as Bingham fluids: some cements, slurries, paints, and biological fluids might exhibit such a behavior. It is actually a well-known property of paints: if put in large quantities on a vertical wall, the paint will flow, whereas if put as a very thin film on the same wall, the paint will not flow, but stay in place, and dry to form a nice colored covering.

Preferred Orientation of the Particles of Fluid

Fluids with properties as above, Newtonian or non-Newtonian, are isotropic in nature, even though they are constituted of atoms, or of long chains of material. They are the same everywhere, optically,

magnetically, or electrically. Some fluids, liquid crystals, or polymeric liquid crystals in particular, have remarkable properties of nonanisotropy, being able to orient themselves, on average, along a particular direction: this is the nematic phase, which is used in many devices (screens for clocks, hand calculators, and cell phones), because the average orientation may be changed by applying an electric field. Other phases of liquid crystals include smectic A, C, and C* phases, where one sees a preferred orientation (tilted for C phases) of the fluid, and also a layer-like structure. As an example, let us mention discotic nematic liquid crystals, which are precursors for carbon-based materials, such as fibers, composites, and films, which possess excellent mechanical and thermal properties. Sails for race sailing boats are made of Kevlar, which is one of these new materials with remarkable properties.

Modeling

The flowing fluid will be described by its (Eulerian) velocity at time t and position x, say $u(x,t)$, for x belonging to the domain of the flow Ω and the time t to $\mathbb{R}_+$, by its mass density $\rho(x,t)$, its pressure $p(x,t)$ ($p>0$ defined up to an additive constant), and its stress $\sigma(x,t)$ – which is a symmetric tensor.

The partial differential equations describing the flow are satisfied in the domain of the flow and read as follows:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0$$
$$\rho\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u\right) = \operatorname{div}\sigma + f \qquad [2]$$

where f denotes some external forces applied to the fluid. These equations describe the conservation of mass and the conservation of linear momentum. To close the system, we need a constitutive equation for the stress σ as well as initial conditions and boundary conditions.

Moreover, most non-Newtonian fluids are practically incompressible in most regions of the flow, so that we shall only consider this case: the first equation in [2] is replaced by condition $\operatorname{div} u = 0$ in the domain of the flow.

Notions of Continuum Mechanics

At time t, a body S occupies a region Ω_t of the Euclidean space $\mathcal{E}_3$, called the configuration at time t, of the body. Points p of S are called material points or particles of fluids. The configuration Ω_t is assumed to be regular in the following sense: Ω_t is closed, its interior is connected and dense everywhere, its boundary is piecewise regular, $\mathcal{C}^0$ at least.

A mapping $\Phi : \Omega_0 \longrightarrow \Omega_t$ is a deformation if Φ is a bijection from Ω_0 onto Ω_t and is a $\mathcal{C}^1$–diffeomorphism from the interior of Ω_0 onto the interior of Ω_t, with positive Jacobian.

The motion of a body S is given by a set of deformations $\Pi(t,t') : \Omega_t \longrightarrow \Omega_{t'}$, satisfying

$$\Pi(t,t) = \mathrm{Id}, \quad \Pi(t'',t) = \Pi(t'',t') \circ \Pi(t',t)$$

The trajectory of the material point which is in X at t_0 is the set

$$\{\Pi(t,t_0)(X), t \geq t_0\}$$

A body is said to be rigid if the deformation $\Pi(t,t')$ is an isometry for all times t and t'. A material point p is said to be attached to the rigid body S if the body $p \cup S$ is rigid.

The motion of a fluid might be described in terms of the Lagrangian coordinates $X \in \Omega_0$ of each particle of fluid: Ω_0 is called the reference configuration and is the fixed configuration occupied by the body of fluid at the time of reference, say t_0. The motion of the fluid might also by described in terms of the Eulerian coordinates $x = \chi(X,t)$, which represent the position of a particle at time t which has position X at t_0. The Lagrangian and Eulerian coordinates of the same particle of fluid are linked by the differential equation

$$\dot{\chi}(X,t) = u((X,t),t), \quad \text{for}\, t \geq t_0$$
$$\chi(X,t_0) = X$$

For defining the constitutive equations, we shall use a few tensors that we define now. The deformation gradient is defined by $F(X,t) = \partial\chi(X,t)/\partial X$, and the right Cauchy–Green tensor by $C = F^{\mathrm{T}}F$ (also called Cauchy strain). To define relative tensors, we denote by $\chi = \chi_t(x,s)$ the position at time $s \leq t$ of the material point, which is at x at time t. The relative tensors are defined in the following way:

- the relative deformation gradient $F_t(s) = \nabla\chi_t(x,s)$,
- the relative right Cauchy–Green tensor $C_t(s) = F_t^{\mathrm{T}}(s) F_t(s)$, and
- the relative Finger tensor $C_t(s)^{-1}$.

Note that the rate of deformation tensor is obtained as the time derivative of the relative Cauchy strain tensor:

$$D = \frac{1}{2}\frac{\partial C_t(s)}{\partial s}\Big|_{s=t}$$

Principle of Objectivity and Frame Invariance

A frame of reference is defined in the spacetime $\mathcal{E}_3 \times \mathbb{R}$ attached to the observer by giving a chronology and a system of reference. The chronology is a timescale, which will be assumed to be the same for all observers. The system of reference is a set of at least four points attached to a rigid body (this is the observer), which are not coplanar.

The constitutive equation needs to satisfy the principle of frame invariance and of frame indifference (or objectivity), which means that the equation does not depend on rigid motions of the observer. In the mathematical framework, it means that the equation has to be invariant under a change of orthonormal frame of reference $x^* = Q(t)x$, where $Q(t)$ is an orthogonal tensor: the transformed equation has to have the same expression, and also to be frame indifferent. We define a scalar quantity φ, a vector field u, or a tensor field τ, as being frame indifferent if, under the change of variables $x^* = Q(t)x$, they satisfy the relations $\varphi(x,t) = \varphi^*(x,t)$, $u(x,t) = Q(t)^{\mathrm{T}} u^*(x^*,t)$, and $\tau(x,t) = Q(t)^{\mathrm{T}} \tau^*(x^*,t)Q(t)$, respectively.

The velocity gradient ∇u is not frame indifferent, but its symmetric part is. The vorticity, which is the antisymmetric part $W = (\nabla u - \nabla u^{\mathrm{T}})/2$ of the velocity gradient, satisfies the equation $\dot{W} = Q^{\mathrm{T}} W^* Q - Q^{\mathrm{T}} \dot{Q}$, where the dot denotes the convective derivative $\mathrm{d}/\mathrm{d}t = \partial/\partial t + (u \cdot \nabla)$.

Note that the convective derivative of a scalar function φ is frame indifferent, which means that

$$\frac{\partial \varphi}{\partial t} + (u \cdot \nabla)\varphi = \frac{\partial \varphi^*}{\partial t} + (u^* \cdot \nabla_*)\varphi^*$$

but the convective derivative of a vector or a tensor is not frame indifferent.

It can be easily checked that the derivative

$$\frac{\mathcal{D}_0 \tau}{\mathcal{D}t} = \frac{\mathrm{d}\tau}{\mathrm{d}t} + \tau W - W\tau \qquad [3]$$

of a (frame-indifferent) tensor τ is frame indifferent, which means that

$$\frac{\mathcal{D}_0 \tau}{\mathcal{D}t} = Q^{\mathrm{T}} \frac{\mathcal{D}_0^* \tau^*}{\mathcal{D}t} Q$$

To obtain another frame-indifferent derivative of a tensor τ, we need to start with the expression [3], to which we may add other terms containing frame-indifferent quantities, for example, combinations of τ and D. A derivative which is often considered is the Oldroyd derivative, as introduced by Oldroyd in 1958:

$$\frac{\mathcal{D}_a \tau}{\mathcal{D}t} = \frac{\mathrm{d}\tau}{\mathrm{d}t} + \tau W - W\tau - a(D\tau + \tau D) \qquad [4]$$

where a is a real parameter, chosen in the interval $[-1, 1]$. (This restriction on a is necessary for viscometric reasons, and obtained when simple flows, such as Couette or Poiseuille flows, are studied.)

The case $a = 1$ corresponds to the upper convected derivative, and the case $a = -1$ to the lower convected derivative. The case $a = 0$ refers to the corotational or Jaumann derivative. Derivatives corresponding to cases $a = -1, 0$, or 1 might actually be obtained by derivating τ in a frame fixed locally to the body of fluid, and which rotates and/or deforms with the body. Moreover, we shall see that the derivatives corresponding to $a = 1$ or -1 have very simple integral expressions.

Constitutive Equations

The constitutive equation of a non-Newtonian fluid is a nonlinear relationship between the stress tensor and objective variables depending on the flow, such as the pressure, the rate of deformation, frame-indifferent derivatives of such quantities, etc.

Analogously to the constitutive equation for an incompressible Newtonian fluid, we may also write the stress tensor in the form $\sigma = -pI + \tau$. The extra stress tensor τ could be either a function of objective variables, which characterize the flow, or defined by a differential equation or by an integral equation. The point here is to model the fact that the fluid might have some elasticity or some memory, or might experience, for example, yield stress or orientational properties.

Shear dependent viscosity fluids A very simple generalization of the incompressible Newtonian fluid consists in making the viscosity dependent on the rate of deformation tensor, $\eta = \eta(D)$. This generalization has been introduced by O A Ladyzhenskaya in 1970 and, if the function is chosen properly, this model reproduces the behavior of existing fluids, at least in certain parts of their flow. For power-law fluids, the viscosity depends on the second invariant $\mathbb{I}_{\mathrm{D}} = (1/2)\mathrm{tr}\, D^2$ of the symmetric tensor D (the first invariant $\mathrm{tr}\, D$ is zero because of incompressibility), and reads as

$$\eta(D) = \eta_0 + m\mathbb{I}_{\mathrm{D}}^{n-1} \qquad [5]$$

where $\eta_0 \geq 0$, $m > 0$, and $n \geq 0$. If $n = 1$, we recover the Newtonian case, whereas for $n < 1$ this equation describes a shear thinning fluid, and for $n > 1$ a shear thickening fluid. The power law is not valid for $\mathbb{I}_{\mathrm{D}}$

close to 0, so that the Carreau–Yasuda law is preferred:

$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = \left(1 + (\lambda \mathbb{I}_D)^{2\alpha}\right)^{(n-1)/(2\alpha)} \quad [6]$$

where η_0 is the zero-shear rate viscosity, η_∞ is the infinite-shear rate viscosity, λ a time constant, n a dimensionless power-law index, $n \geq 0$, and $\alpha > 0$ a parameter (generally equal to 1 for a monomolecular polymer).

Oldroyd models and related models Oldroyd models are differential models built with one of the Oldroyd derivatives, and are very commonly used for polymer solutions or melts. The stress tensor is given as a solution of a differential equation in the following way:

$$\tau + \lambda_1 \frac{\mathcal{D}_a \tau}{\mathcal{D}t} + g(\tau, D) = 2\eta \left(D + \lambda_2 \frac{\mathcal{D}_a D}{\mathcal{D}t} \right) \quad [7]$$

where $\lambda_1 > 0$ is a relaxation time, λ_2 is a retardation time, $0 \leq \lambda_2 < \lambda_1$, and $g(\tau, D)$ is a tensor-valued function, constrained to certain restrictions due to objectivity, and which is at least quadratic.

The Johnson–Segalman model has $g = 0$, and $-1 \leq a \leq 1$. Other models of differential type often suppose the parameter a to be 1, because it has been noticed that with a close to 1 the model is able to reproduce some experimental behavior, whereas for $a = -1$ or close to -1, the model does not work at all. Among the models with $a = 1$, the following ones are fairly popular: the model of Phan-Thien and Tanner has $g(\tau, D) = \alpha\tau \operatorname{tr} \tau$, where α is a constant; this model can be generalized by defining $g(\tau, D) = \alpha\tau^2 + \beta\tau, \alpha$ and β being functions of the trace of τ and of its determinant; the model of Giesekus is the particular case where α is a constant and $\beta = 0$. The Oldroyd eight-constant model is given by

$$g(\tau, D) = \mu_0(\operatorname{tr} \tau) D + \nu_1 \operatorname{tr}(\tau D) I + \mu_2 D^2 + \nu_2 \operatorname{tr}(D^2) I$$

where μ_0, ν_1, μ_2, and ν_2 are constants.

In [7], the limit case $\lambda_2 = 0$ corresponds to Maxwell's type models, where there is no Newtonian viscosity, while the case $\lambda_2 > 0$ corresponds to the Jeffreys' type models. The cases where $a = 1$ and $g = 0$, are often considered in mathematical or numerical studies: this is the upper convected Maxwell (UCM) model for $\lambda_2 = 0$, and the Oldroyd B model for $\lambda_2 > 0$.

The parameters λ_1, λ_2, and η might also depend on $\mathbb{I}_D$: such a model where the upper convected derivative ($a = 1$) is chosen is referred to as the White–Metzner model, and reads as follows:

$$\tau + \lambda_\mathbb{I} \frac{\mathcal{D}_1 \tau}{\mathcal{D}t} = 2\left(\eta_\mathbb{I} D + \eta_\infty \left(D + \lambda_\mathbb{I} \frac{\mathcal{D}_1 D}{\mathcal{D}t} \right) \right)$$

where η_∞ is also the Newtonian viscosity.

Integral equations Other constitutive equations for viscoelastic fluids include integral equations. Actually, some differential equations have integral counterparts: this is the case for the differential equations associated with the upper or lower convected frame-indifferent derivatives. For the upper convected derivative ($a = 1$), the extra stress is given by the integral expression

$$\tau(x, t) = 2\eta \frac{\lambda_2}{\lambda_1} D(x, t) + 2\eta \frac{\lambda_1 - \lambda_2}{\lambda_1^2} \times \int_{-\infty}^{t} e^{-(t-s)/\lambda_1} (\nabla_X x) D(X, s) (\nabla_X x)^{\mathrm{T}} \, ds$$

where X is the position, at time s, of the point which is at x at time t. A similar expression might be obtained for the lower convected derivative.

A very common integral equation is the K–BKZ equation (introduced independently by Kaye and Bernstein, Kearsley, and Zapas in 1962–63). In a simplified form, the extra-stress tensor is given as the integral of a combination of the relative Cauchy strain tensor C_t and its inverse:

$$\tau(x, t) = 2 \int_{-\infty}^{t} G(t - s) \left[\frac{\partial \mathcal{W}(I_1, I_2)}{\partial I_1} C_t^{-1}(s) - \frac{\partial \mathcal{W}(I_1, I_2)}{\partial I_2} C_t(s) \right] ds$$

where $I_1 = \operatorname{tr} C_t^{-1}(s)$ and $I_2 = \operatorname{tr} C_t(s)$. The function G is a given kernel, and $\mathcal{W}$ a given scalar potential. The upper convected Maxwell model is obtained from the K–BKZ model by setting $\mathcal{W}(I_1, I_2) = I_1$ and $G(s) = (\lambda_1 \lambda_2 / 2) \, e^{-\lambda_1 s}$.

Models issued from kinetic theories or micro–macro models Polymeric fluids could also be modeled by coupling a macroscopic viewpoint – the one of continuum mechanics, as described above – and a microscopic viewpoint. A polymer is, in general, made of long chains of molecules. Rather than trying to represent the polymer behavior by a sophisticated constitutive equation, one describes the mean behavior of the molecules by using their microscopic description.

To take an example, we consider a dilute solution of polymer, where each chain of polymer is modeled as a collection of dumbbells, each of them consisting of two beads connected by a spring. The configuration of the spring, namely its length and orientation, is described by a random vector field $Q \in \mathbb{R}^3$. The dumbbells are convected and stretched by the flow.

The probability $\psi(x, Q, t)\,dQ$ of finding a dumbbell with a configuration Q at (x, t) is governed by a Fokker–Planck equation:

$$\frac{d\psi}{dt} + \mathrm{div}_Q((\nabla u)Q\psi) = \frac{2}{\zeta}\,\mathrm{div}_Q((\nabla_Q \mathcal{W})\psi) + \frac{2kT}{\zeta}\Delta_Q\psi$$

where ζ is the friction coefficient of the dumbbell beads, T the temperature, and k the Planck constant, and $\mathcal{W}$ the spring potential. The extra stress is given by the constitutive equation

$$\tau = \lambda \int (\nabla_Q \mathcal{W} \otimes Q)\psi(x, Q, t)\,dQ$$

The simplest potential is the linear one (also called Hookean potential) $\mathcal{W}(Q) = H|Q|^2$, where $|Q|$ is the length of Q, and H the elasticity constant. In fact, in the case of the Hookean potential, this set of equations is equivalent to the Oldroyd B model. Another potential corresponds to finitely extendable nonlinear elastic (FENE) chain of dumbbells,

$$\mathcal{W}(Q) = -\frac{HQ_0^2}{2}\log\left(1 - \frac{|Q|^2}{Q_0^2}\right)$$

for $|Q| \leq Q_0$, and gives the FENE model, for which there is no macroscopic constitutive equation known.

We have only made here a short incursion in these micro–macro models: research is in progress, both analytical and numerical (Öttinger 1996, Suen *et al.* 2002, Keunings 2004).

Liquid crystals and polymeric liquid crystals As an example, we present the constitutive equations for a uniaxial nematic liquid crystal.

In the theory of Leslie and Ericksen, established in the 1960s and the 1970s, the stress tensor is given as a function of the orientation unit vector n, through the Oseen–Frank elastic energy,

$$2\mathcal{W}(n, \nabla n) = \kappa_1(\mathrm{div} n)^2 + \kappa_2(n \cdot \mathrm{curl}\, n)^2 + \kappa_3|n \times \mathrm{curl}\, n|^2$$

where $\kappa_1 > 0, \kappa_2 > 0$, and $\kappa_3 > 0$ are the three basic modes (splay, twist, and bend, respectively). The extra stress tensor is precisely given by the relation

$$\tau = -(\nabla n)^{\mathrm{T}}\frac{\partial \mathcal{W}}{\partial \nabla n} + \alpha_1(n \cdot \boldsymbol{D}n)n \otimes n + \alpha_2 \boldsymbol{N} \otimes n + \alpha_3 n \otimes \boldsymbol{N} + \alpha_4 \boldsymbol{D} + \alpha_5 \boldsymbol{D}n \otimes n + \alpha_6 n \otimes$$

where $\boldsymbol{N} = \dot{n} - \boldsymbol{W}n$ is the corotational derivative of the director, and $\alpha_i, i = 1, \ldots, 6$, the six Leslie viscosity coefficients.

The director satisfies a differential equation derived from continuum mechanics,

$$\rho_1 \ddot{n} = G + g + \mathrm{div}\pi$$

where ρ_1 is the moment of inertia per unit volume, G the external director body force (torque per unit volume), π the director stress tensor, and g the intrinsic director body force. Precisely,

$$g = \lambda n - (\nabla n)\beta - \frac{\partial \mathcal{W}}{\partial n} - \gamma_1 \boldsymbol{N} - \gamma_2 \boldsymbol{D}n$$

$$\pi = n \otimes \beta + \frac{\partial \mathcal{W}}{\partial \nabla n}$$

where β is a Lagrange multiplier vector, and $\lambda = -\gamma_2/\gamma_1$ is the reactive parameter, with $\gamma_1 = \alpha_3 - \alpha_2$ the rotational viscosity, and $\gamma_2 = \alpha_6 - \alpha_5 = \alpha_3 + \alpha_2$ the irrotational torque coefficient.

Polymeric liquid crystals might have other variables entering in the modeling, such as order parameters, order tensors, etc.

Because of the complexity of modeling, most studies concern either very simple flows, such as Couette or Poiseuille flows, or steady flows, or flows for which the coefficients satisfy specific relationships.

Reports about earlier studies, theoretical as well as numerical, can be found in Coron *et al.* (1991), and references therein. The study of polymeric liquid crystals, or of the smectic phase of liquid crystals is at its very early stage and one could look into it in specialized journals, such as the *Journal of Non-Newtonian Fluid Mechanics*, or *see* Liquid Crystals.

Yield stress fluids Bingham materials have the property of flowing only when the stress magnitude is greater than a critical value, and being a solid otherwise. Precisely, in the simplest and the most widely used model, the Bingham model, the extra stress tensor τ is given by the relations

$$\begin{aligned} \tau &= 2\eta \boldsymbol{D} + \tau_* \frac{\boldsymbol{D}}{\mathbb{I}_{\mathrm{D}}} && \text{if } \mathbb{I}_{\mathrm{D}} \neq 0 \\ |\tau| &\leq \tau_* && \text{if } \mathbb{I}_{\mathrm{D}} = 0 \end{aligned} \qquad [8]$$

where $\tau_* > 0$ is the yield limit. The Bingham model is generalized in taking the viscosity η to be a function of the shear stress: η is given by the relation

$$\eta = 1 + 2\left(\frac{\tau_*}{\mathbb{I}_{\mathrm{D}}}\right)^{1/2}$$

for the Casson law, and by the power law [5] for the Herschel–Bulkley model.

The mathematical study was started by Duvaut and Lions (1976), and regained interest recently (Malek and Rajagopal 2005), especially in relation with other recent studies in polymeric liquids.

Theoretical and Numerical Problems for Viscoelastic Flows

The mathematical study of viscoelastic fluid flows amounts to studying systems of partial differential equations, which all include either the incompressible Euler equation or the incompressible Navier–Stokes equation as particular cases. In particular, it means that the results obtained from such a study are similar to the ones obtained for Euler or Navier–Stokes equations, and, because of the complexity of the system, the results are expected to be qualitatively as good, actually more often less good, than for these equations. For example, the existence of weak three-dimensional solutions to the Navier–Stokes system is known, while for non-Newtonian flows, this result will be true only in very specific cases. Moreoever, when a result is not known for the Navier–Stokes problem, such as the uniqueness of solution for all data in a three-dimensional problem, there is no hope something similar could be proved for non-Newtonian fluid flows.

As an example, we consider the case of Johnson–Segalman fluids, which are described by constitutive equation [7] with $g=0$. Recall that the limit case $\lambda_2=0$ corresponds to the purely elastic case, and $\lambda_2=\lambda_1$ to the purely Newtonian case. Equation [7] is coupled with the equations of motion:

$$\rho\frac{\mathrm{d}u}{\mathrm{d}t}+\nabla p=\operatorname{div}\tau+f \qquad \operatorname{div}u=0 \tag{9}$$

Equations [7] and [9] have to be solved in the domain of the flow, which might be the whole space $\mathbb{R}^3$ (or $\mathbb{R}$ or $\mathbb{R}^2$ in case of symmetries), or a domain Ω, bounded or not, in $\mathbb{R}^n$, $n=1$, 2, or 3. These equations are supplemented by appropriate boundary conditions and initial conditions for the velocity u and the extra stress τ (no boundary condition on τ is needed if the homogeneous nonslip boundary condition $u=0$ is chosen).

We first make explicit the Newtonian contribution to the stress by setting $\tau=\tau^{\mathrm{s}}+\tau^{\mathrm{p}}$ and $\tau^{\mathrm{s}}=2\eta_{\mathrm{s}}\boldsymbol{D}$. The differential equation for τ^{p} is then

$$\tau^{\mathrm{p}}+\lambda_1\frac{\mathcal{D}_a\tau^{\mathrm{p}}}{\mathcal{D}t}=2\eta_{\mathrm{p}}\boldsymbol{D}$$

where $\eta_{\mathrm{p}}=(1-\lambda_2/\lambda_1)\eta$ is the so-called polymeric viscosity, $\eta_{\mathrm{s}}=(\lambda_2/\lambda_1)\eta$ the so-called Newtonian viscosity (or solvent viscosity).

We then use nondimensional variables, so as to make explicit the characteristic parameters, which the flow depends on. The non-Newtonian fluid considered in this model will always be homogeneous: its density ρ is a constant independent of x and t. The dimensional variables are now asterisked. We define quantities which are characteristic of the flow: a length L, a velocity magnitude U, a stress magnitude T, a force magnitude F, and a pressure P. We operate the change of variables and functions $x=x^*/L$, $u=u^*/U$, $t=Ut^*/L$, and also introduce the nondimensional functions

$$\tau=\frac{\tau^*}{T},\quad p=\frac{p^*}{P},\quad f=\frac{f^*}{F}$$

After choosing the parameters T, P, and F in an appropriate way, namely $T=P=\eta U/L$, and $F=\eta U/L^2$, we obtain the following system

$$\begin{aligned} Re\frac{\mathrm{d}u}{\mathrm{d}t}+\nabla p&=(1-\omega)\Delta u+\operatorname{div}\tau+f\\ \operatorname{div}u&=0\\ We\frac{\mathcal{D}_a\tau}{\mathcal{D}t}+\tau&=2\omega\boldsymbol{D}\end{aligned} \tag{10}$$

Here the three nondimensional parameters which the flow depends on are the usual Reynolds number $Re=\rho_0UL/\eta$ and two other numbers: the Weissenberg number $We=\lambda U/L$ measures the elasticity per unit time (sometimes also called the Deborah number), and the parameter $\omega=\eta_{\mathrm{p}}/\eta$ is the ratio of elastic viscosity to total viscosity ($\omega=0$ corresponds to the Newtonian case, while $\omega=1$ corresponds to the purely elastic case).

System [10] couples a transport equation (the equation for the stress τ), and either a Navier–Stokes type equation when $\omega<1$, or a Euler type equation when $\omega=1$ (for the velocity u). This system is not hyperbolic, parabolic, or elliptic.

Maxwell's type models ($\omega=1$) display two striking phenomena. First, the Cauchy problem (with initial data) can present Hadamard instabilities, that is, instabilities to short waves. It means, in particular, that the Cauchy problem is not well posed in any good class but analytic. Moreover, the partial differential system for Maxwell's type steady flows may experience a change of type, analogous to the situation in gas dynamics, if the "Mach number" $Re\,We$ is larger than 1.

Jeffreys' type models ($\omega<1$), because of the presence of a Newtonian viscosity, do not exhibit such phenomenon, but their study does not enter in

the theory of parabolic equations either, the type of the system being composite.

Problems of interest for rheologists, as well as for mathematicians, include in particular the high Weissenberg asymptotics, the high Weissenberg boundary layers, the singularity of flows near a reentrant corner, and the stability of flows.

We give a few details about stability questions. Instabilities are seen in experimental extrusion of melted polymers from a pipe: melt fracture designates different phenomena appearing at different stages of the experiment, when the speed of the extrusion is increased, such as sharkskin instability, slight distortions of the extrudate, large distortions and wavyness of the extrudate. One may distinguish two kinds of instabilities. First, constitutive instabilities are associated with nonmonotonicity of constitutive functions and loss of evolutionary property of the equations of motion. Other kinds of instabilities are close to classical hydrodynamic instabilities at increasing *Re*. Note that in viscoelastic flows the *Re* is usually very small, and might even be set to zero in some studies.

Other mathematical questions for system [10] include existence of weak solutions (for the very special case of Oldroyd model with the Jaumann derivative where ($a = 0$) in [5]), existence of regular solutions defined on some time interval, depending on the magnitude of the data, and existence of regular solutions for all times. Other studies concern the existence, uniqueness, and stability of steady solutions. Another field of study is the numerical simulation of such flows.

In summary, there have been numerous computations made in the field of steady or unsteady viscoelastic fluids, and especially models using continuum mechanics. Standard test problems include the cavity-driven flow, flows inside a 4 : 1 contraction, extrusion flows, flows between eccentric cylinders, and flows in "wiggly" pipes. As mentioned already, the type of the sytem of partial differential equations is composite, neither elliptic nor hyperbolic. The numerical codes have to take into account the precise nature of the set of partial differential equations, so as to be able to obtain noncatastrophic results. One of the main challenges has been to deal with the high-*We* problem: with increasing *We*, the results would become totally incoherent, and the numerical algorithms would diverge.

Nowadays, with the power of computers increasing, molecular simulations of flows are proposed, using the macro–micro modeling mentioned above. Also, simulations of flows of colloidal suspensions and reacting flows have been undertaken with success.

See also: Compressible Flows: Mathematical Theory; Fluid Mechanics: Numerical Methods; Incompressible Euler Equations: Mathematical Theory; Interfaces and Multicomponent Fluids; Inviscid Flows; Liquid Crystals; Newtonian Fluids and Thermohydraulics; Partial Differential Equations: Some Examples; Stability of Flows; Stochastic Hydrodynamics; Viscous Incompressible Fluids: Mathematical Theory.

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Nonperturbative and Topological Aspects of Gauge Theory

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Introduction

Classical fields that enter a classical field theory provide a mapping from the "base" manifold on which they are defined (space or spacetime) to a "target" space over which they range. The base and target spaces, as well as the map, may possess nontrivial topological features, which affect the fixed-time description and the temporal evolution of the fields, thereby influencing the physical reality that these fields describe. Quantum fields of a quantum field theory are operator-valued distributions whose relevant topological properties are obscure. Nevertheless, topological features of the corresponding classical fields are important in the quantum theory for a variety of reasons: (1) Quantized fields can undergo local (spacetime-dependent) transformations (gauge transformations, coordinate diffeomorphisms) that involve classical functions whose topological properties determine the allowed quantum field theoretic structures. (2) One formulation of the quantum field theory uses a functional integral over classical fields, and classical topological features become relevant. (3) Semiclassical (WKB) approximations to the quantum theory rely on classical dynamics, and again classical topology plays a role in the analysis.

Topological effects of gauge fields in quantum theory were first appreciated by Dirac in his study of the quantum mechanics for (hypothetical) magnetic point monopoles. Although here one is not dealing with a field theory, the consequences of his analysis contain many features that were later encountered in field theory models.

The Lorentz equations of motion for a charged (e) massive (M) particle in a monopole magnetic field ($\boldsymbol{B}=m\boldsymbol{r}/r^3$) are unexceptional,

$$\dot{\boldsymbol{r}} = \frac{\boldsymbol{p}}{M} \qquad [1a]$$

$$\dot{\boldsymbol{p}} = \frac{e}{M}\boldsymbol{p}\times\boldsymbol{B} \quad (c=1) \qquad [1b]$$

and completely determine classical dynamics. But knowledge of the Lagrangian L and of the action I – the time integral of L: $I=\int \mathrm{d}t\, L$ – is further needed for quantum mechanics, either in its functional integral formulation or in its Hamiltonian formulation, which requires the canonical momentum $\boldsymbol{\pi}\equiv \partial L/\partial\dot{\boldsymbol{r}}$. The Lorentz-force action is expressed in terms of the vector potential $\boldsymbol{A}$, $\boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}$: $I_{\mathrm{Lorentz}}=e\int \mathrm{d}t\,\dot{\boldsymbol{r}}\cdot\boldsymbol{A}=e\int \mathrm{d}\boldsymbol{r}\cdot\boldsymbol{A}$. The magnetic monopole vector potential is necessarily singular because $\boldsymbol{\nabla}\cdot\boldsymbol{B}=4\pi m\delta^3(\boldsymbol{r})\neq 0$. The singularity (Dirac string) can be moved, but not removed, by gauge transformations, which also are singular, and do not leave the Lorentz action invariant. Noninvariance of the action can be tolerated provided its change is an integral multiple of 2π, since the functional integrand involves exp (iI) (with $\hbar=1$). The quantal requirement, which is not seen in the equations of motion, is met when

$$eg = N/2 \qquad [2]$$

The topological background to this (Dirac) quantization condition is the fact that $\Pi_1(\mathrm{U}(1))$ is the group of integers, that is, the map of the unit circle into the gauge group, here U(1), is classified by integers.

Further analysis shows that only point magnetic sources can be incorporated in particle quantum mechanics, which is governed by the particle Hamiltonian $H=\boldsymbol{p}^2/2M$ (magnetic fields do no work and are not seen in H). Quantum Lorentz equations are regained by commutation with H: $\dot{\boldsymbol{r}}=\mathrm{i}[H,\boldsymbol{r}]$, $\dot{\boldsymbol{p}}=\mathrm{i}[H,\boldsymbol{p}]$, provided

$$\mathrm{i}[r^i, r^j] = 0 \qquad [3a]$$

$$\mathrm{i}[p^i, r^j] = \delta^{ij} \qquad [3b]$$

$$\mathrm{i}[p^i, p^j] = -e\varepsilon^{ijk}B^k \qquad [3c]$$

But [3c] implies that the Jacobi identity is obstructed by magnetic sources $\boldsymbol{\nabla}\cdot\boldsymbol{B}\neq 0$.

$$\tfrac{1}{2}\varepsilon^{ijk}[p^i,[p^j,p^k]] = e\boldsymbol{\nabla}\cdot\boldsymbol{B} \qquad [4]$$

This obstruction is better understood by examining the unitary operator $U(\boldsymbol{a})\equiv \exp(\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p})$, which according to [3b] implements finite translations of $\boldsymbol{r}$ by $\boldsymbol{a}$. The commutator algebra [3] and the failure of the Jacobi identity [4] imply that these operators do not associate. Rather one finds

$$U(\boldsymbol{a}_1)(U(\boldsymbol{a}_2)U(\boldsymbol{a}_3)) = \mathrm{e}^{\mathrm{i}\Phi}(U(\boldsymbol{a}_1)U(\boldsymbol{a}_2))U(\boldsymbol{a}_3) \qquad [5]$$

where $\Phi=e\int \mathrm{d}^3x\,\boldsymbol{\nabla}\cdot\boldsymbol{B}$ is the total flux emerging from the tetrahedron formed from the three vectors $\boldsymbol{a}_i$ with vertex at $\boldsymbol{r}$ (see **Figure 1**). But quantum mechanics realized by linear operators acting on a Hilbert space requires that operator multiplication

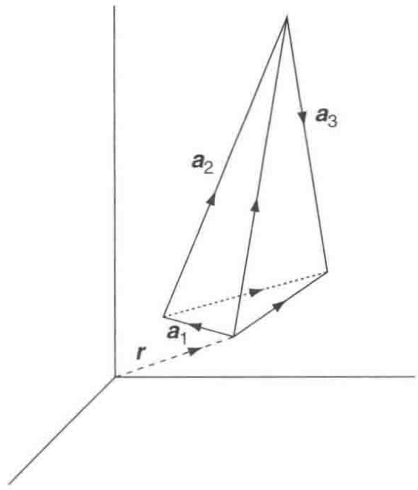


Figure 1 Tetrahedron pierced by magnetic flux that obstructs associativity.

be associative. This can be achieved, in spite of [5], provided Φ is an integral multiple of 2π, hence invisible in the exponent. This then needs that (1) $\nabla \cdot \boldsymbol{B}$ be localized at points, so that the volume integral of $\nabla \cdot \boldsymbol{B}$ retain integrality for arbitrary $\boldsymbol{a}_i$ and (2) the strengths of the localized poles obey Dirac quantization. The points at which $\nabla \cdot \boldsymbol{B}$ is localized can now be removed from the manifold and the Jacobi identity is regained. The above argument, which rederives Dirac's quantization, makes no reference to gauge variance of magnetic potentials.

In the remainder we shall discuss related phenomena for selected gauge field theories in four, three, and two dimensions that describe actual physical events occurring in nature. We shall encounter in generalized form, analogs to the above quantum mechanical system.

Some definitions and notational conventions: Nonabelian gauge potentials A_μ^a carry a spacetime index (μ) (metric tensor $g_{\mu\nu} = \mathrm{diag}(1, -1, \ldots)$) and an adjoint group index (a). When contracted with anti-Hermitian matrices T_a that represent the group's Lie algebra (structure constants $f_{ab}{}^c$)

$$[T_a, T_b] = f_{ab}{}^c T_c \qquad [6]$$

they become Lie algebra-valued.

$$A_\mu \equiv A_\mu^a T_a \qquad [7]$$

Gauge transformations transform A_μ by group elements U:

$$A_\mu \to A_\mu^U \equiv U^{-1} A_\mu U + U^{-1} \partial_\mu U \qquad [8a]$$

For infinitesimal gauge transformations, $U \approx I + \lambda$, $\lambda \equiv \lambda^a T_a$; this leads to the covariant derivative D_μ:

$$\begin{aligned} A_\mu &\to A_\mu + \partial_\mu \lambda + [A_\mu, \lambda] \equiv A_\mu + D_\mu \lambda \\ A_\mu^a &\to A_\mu^a + \partial_\mu \lambda^a + f_{bc}{}^a A_\mu^b \lambda^c \equiv A_\mu^a + (D_\mu \lambda)^a \end{aligned} \qquad [8b]$$

(In a quantum field theory, A_μ becomes an operator but the gauge transformations U, λ remain c-number functions.) The field strength $F_{\mu\nu}$ given by

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] \qquad [9a]$$

is also given by

$$[D_\mu, D_\nu] \ldots = [F_{\mu\nu}, \ldots] \qquad [9b]$$

(coupling strength g has been scaled to unity). The definition [9] implies the Bianchi identity

$$D_\mu F_{\nu\omega} + D_\omega F_{\mu\nu} + D_\nu F_{\omega\mu} = 0 \qquad [10]$$

Here $F_{\mu\nu}$ is gauge covariant

$$F_{\mu\nu} \to F_{\mu\nu}{}^U = U^{-1} F_{\mu\nu} U \qquad [11a]$$

or, infinitesimally,

$$F_{\mu\nu} \to F_{\mu\nu} + [F_{\mu\nu}, \lambda] \qquad [11b]$$

In the gauge invariant Yang–Mills action I_{YM}, the Yang–Mills Lagrange density $\mathcal{L}_{\mathrm{YM}}$ is integrated over the base space,

$$\begin{aligned} \mathcal{L}_{\mathrm{YM}} &= \tfrac{1}{2} \mathrm{tr}\, F^{\mu\nu} F_{\mu\nu} \\ I_{\mathrm{YM}} = \int \mathcal{L}_{\mathrm{YM}} &= \frac{1}{2} \int \mathrm{tr}\, F^{\mu\nu} F_{\mu\nu} \end{aligned} \qquad [12]$$

The trace is evaluated with the convention

$$\mathrm{tr}\, T_a T_b = -\tfrac{1}{2} \delta_{ab} \qquad [13]$$

and henceforth there is no distinction between upper and lower group indices. The Euler–Lagrange condition for stationarizing I_{YM} gives the Yang–Mills equation

$$D_\mu F^{\mu\nu} = 0 \qquad [14a]$$

Should sources J^μ be present, [14a] becomes

$$D_\mu F^{\mu\nu} = J^\nu \qquad [14b]$$

and J^μ must be covariantly conserved:

$$\begin{aligned} D_\nu J^\nu = D_\nu D_\mu F^{\mu\nu} &= -\tfrac{1}{2} [D_\mu, D_\nu] F^{\mu\nu} \\ &= -\tfrac{1}{2} [F_{\mu\nu}, F^{\mu\nu}] = 0 \end{aligned} \qquad [15]$$

All this is a nonabelian generalization of familiar Maxwell electrodynamics.

Gauge Theories in Four Dimensions

Gauge theories in four-dimensional spacetime are at the heart of the standard particle physics model. Their topological features have physical consequences and merit careful study.

Yang–Mills Theory

In four dimensions, we define nonabelian electric E^a and magnetic B^a fields,

$$E^{ia} = F^a_{0i}, \qquad B^{ia} = -\tfrac{1}{2}\varepsilon^{ijk}F^a_{jk} \qquad [16]$$

Canonical analysis and quantization is carried out in the Weyl gauge ($A^a_0 = 0$), where the Lagrangian and Hamiltonian (energy) densities read

$$\mathcal{L}_{\rm YM} = \tfrac{1}{2}(E^a \cdot E^a - B^a \cdot B^a) \qquad [17]$$

$$\mathcal{H}_{\rm YM} = \tfrac{1}{2}(E^a \cdot E^a + B^a \cdot B^a) \qquad [18]$$

The first term is kinetic, with $E^a = -\partial_t A^a$ also functioning as the (negative) canonical momentum π^a, conjugate to the canonical variable A^a; the second magnetic term gives the potential. In the Weyl gauge, the theory remains invariant against time-independent gauge transformations. The time component of equation [14] (Gauss law) is absent (because there is no A^a_0 to vary); rather it is imposed as a fixed-time constraint on the canonical variables E^a and A^a. This regains the Gauss law:

$$(\mathcal{D} \cdot E)^a = 0 \quad \text{(in the absence of sources)} \qquad [19a]$$

In the quantum theory $\mathcal{D} \cdot E$ annihilates "physical" states. Explicitly, in a functional Schrödinger representation, where states are functionals of the canonical fixed-time variable $A|\Psi\rangle \to \Psi(A)$, [19a] requires

$$\left(\mathcal{D} \cdot \frac{\delta}{\delta A}\right)^a \Psi(A) = 0 \qquad [19b]$$

that is, physical states must be invariant against infinitesimal gauge transformation, or equivalently, against gauge transformations that are homotopic (continuously deformable) to the identity (the so-called "small" gauge transformations)

$$\Psi(A + \mathcal{D}\lambda) = \Psi(A) \qquad [20]$$

But homotopically nontrivial gauge transformation functions that cannot be deformed to the identity (the so-called "large" gauge transformations) may be present. Their effect is not controlled by Gauss' law, and must be discussed separately.

Fixed-time gauge transformation functions depend on the spatial variable $\boldsymbol{r}: U(\boldsymbol{r})$. For a topological classification, we require that U tend to a constant at large r. Equivalently, we compactify the base space R^3 to S^3. Thus, the gauge functions provide a mapping from S^3 into the relevant gauge group G, and for nonabelian compact gauge groups such mappings fall into disjoint homotopy classes labeled by an integer winding number n: $\Pi^3(G) = Z$. Gauge functions U_n belonging to different classes cannot be deformed into each other; only those in the "zero" class are deformable to the identity. An analytic expression for the winding number $\omega(U)$ is

$$\omega(U) = \frac{1}{24\pi^2}\int {\rm d}^3x\, \varepsilon^{ijk}{\rm tr}(U^{-1}\partial_i U U^{-1}\partial_j U U^{-1}\partial_k U) \qquad [21]$$

This is a most important topological entity for gauge theories in four-dimensional spacetime, that is, in 3-space, and we shall meet it again in a description of gauge theories in three-dimensional spacetime, that is, on a plane. Various features of ω expose its topological character: (1) $\omega(U)$ does not involve a metric tensor, yet it is diffeomorphism invariant. (2) $\omega(U)$ does not change under local variations of U:

$$\begin{aligned}\delta\omega(U) &= \frac{1}{8\pi^2}\int {\rm d}^3x\, \partial_i \varepsilon^{ijk}{\rm tr}(U^{-1}\delta U U^{-1}\partial_j U U^{-1}\partial_k U)\\ &= \frac{1}{8\pi^2}\int {\rm d}S^i\, \varepsilon^{ijk}{\rm tr}(U^{-1}\delta U U^{-1}\partial_j U U^{-1}\partial_k U)\\ &= 0\end{aligned} \qquad [22]$$

The last integral is over the surface (at infinity) bounding the base space and vanishes for localized variations δU. In fact, the entire $\omega(U)$, not only its variation, can be presented as a surface integral, but this requires parametrizing the group element U on R^3. For example, for SU(2),

$$\begin{aligned}&U = \exp\lambda, \quad \lambda = \lambda^a\sigma^a/2{\rm i} \quad (\boldsymbol{\sigma} \equiv \text{Pauli matrices})\\ &\omega(U) = \frac{1}{16\pi^2}\int {\rm d}S^i\, \varepsilon^{ijk}\varepsilon_{abc}\hat\lambda^a\partial_j\hat\lambda^b\partial_k\hat\lambda^c(\sin|\lambda| - |\lambda|)\\ &|\lambda| \equiv \sqrt{\lambda^a\lambda^a}, \qquad \hat\lambda^a \equiv \lambda^a/|\lambda|\end{aligned} \qquad [23]$$

Specifically, with $|\lambda| \underset{r\to\infty}{\longrightarrow} 2\pi n$ (so that $U \underset{r\to\infty}{\longrightarrow} \pm I$), $\omega(U) = -n$. As befits a topological entity, $\omega(U)$ is determined by global (here large distance) properties of U.

Since all gauge transformations, small and large, are symmetry operations for the theory, [20] should be generalized to

$$\Psi(A^{U_n}) = {\rm e}^{{\rm i}n\theta}\Psi(A) \qquad [24]$$

where θ is an universal constant. Thus, Yang–Mills quantum states behave as Bloch waves in a periodic lattice, with large gauge transformations playing the role of lattice translations and the Yang–Mills vacuum angle θ playing the role of the Bloch momentum. This is further understood by noting that the profile of the potential energy density, $\frac{1}{2}B^a \cdot B^a$ possesses a periodic structure symbolically depicted in **Figure 2**.

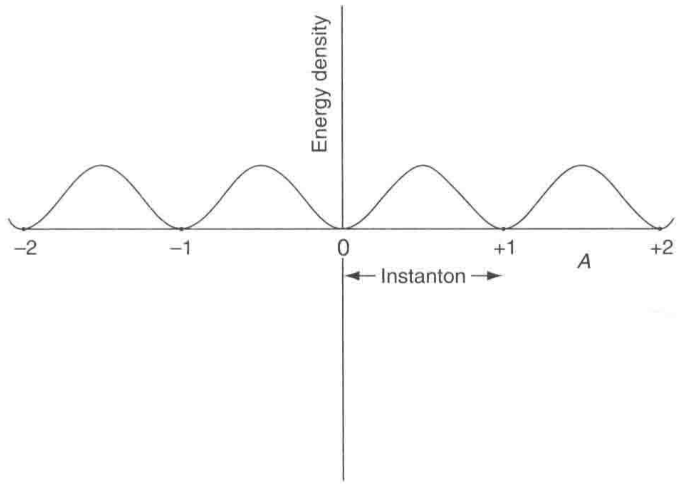


Figure 2 Schematic for energy periodicity of Yang–Mills fields.

Thanks to Gauss' law, potentials A that differ by small gauge transformations are identified, while those differing by large gauge transformations give rise to the periodicity. Zero energy troughs correspond to pure gauge vector potentials in different homotopy classes n: $\mathbf{A} = -U_n^{-1}\nabla U_n$.

The θ angle (Bloch momentum) arises from quantum tunneling in $\mathbf{A}$ space. Usually, in field theory tunneling is suppressed by infinite energy barriers. (This gives rise to spontaneous symmetry breaking.) However, in Yang–Mills theory there are paths in field space that avoid such barriers. Quantum tunneling paths are exhibited in a semiclassical approximation by identifying classical motion in imaginary time (Euclidean space) that interpolates between classically degenerate vacua and possesses finite action.

In Yang–Mills theory, continuation to imaginary time, $x^0 \to ix^4$, places a factor of i on $\mathbf{E}^a$. Zero (Euclidean) energy is maintained when $\mathbf{E}^a = \pm\mathbf{B}^a$, or with covariant notation in Euclidean space,

$$\tfrac{1}{2}\varepsilon^{\mu\nu\alpha\beta}F_{\alpha\beta} \equiv {}^*F^{\mu\nu} = \pm F^{\mu\nu} \qquad [25]$$

Euclidean finite action field configurations that satisfy [25] are called self-dual or anti-self-dual instantons. By virtue of the Bianchi identity [10], instantons also solve the field equation [14a] in Euclidean space. Since the Euclidean action may also be written as

$$I_{\mathrm{YM}} = \frac{1}{4}\int d^4x\, \mathrm{tr}(F^{\mu\nu} \pm {}^*F^{\mu\nu})(F_{\mu\nu} \pm {}^*F_{\mu\nu}) \mp \frac{1}{2}\int d^4x\, \mathrm{tr}\,{}^*F^{\mu\nu}F_{\mu\nu} \qquad [26]$$

and the first term vanishes for instantons, we see that instantons are characterized by the last term, the Chern–Pontryagin index,

$$\mathcal{P} \equiv -\frac{1}{16\pi^2}\int d^4x\, \mathrm{tr}({}^*F^{\mu\nu}F_{\mu\nu}) = -\frac{1}{32\pi^2}\int d^4x\, \varepsilon^{\mu\nu\alpha\beta}\,\mathrm{tr}(F_{\alpha\beta}F_{\mu\nu}) \qquad [27]$$

This again is an important topological entity:

1. The diffeomorphism invariant $\mathcal{P}$ does not involve the metric tensor.
2. $\mathcal{P}$ is insensitive to local variations of A_μ,

$$\delta\mathcal{P} = -\frac{1}{8\pi^2}\int d^4x\, \mathrm{tr}({}^*F^{\mu\nu}\delta F_{\mu\nu}) = -\frac{1}{4\pi^2}\int d^4x\, \mathrm{tr}({}^*F^{\mu\nu}D_\mu\delta A_\nu) = \frac{1}{4\pi^2}\int d^4x\, \mathrm{tr}(D_\mu{}^*F^{\mu\nu}\delta A_\nu) = 0 \qquad [28]$$

3. $\mathcal{P}$ may be presented as a surface integral owing to the formula

$$\tfrac{1}{4}\mathrm{tr}\,{}^*F^{\mu\nu}F_{\mu\nu} = \partial_\mu K^\mu \qquad [29]$$

$$K^\mu \equiv \varepsilon^{\mu\nu\alpha\beta}\,\mathrm{tr}\big(\tfrac{1}{2}A_\alpha\partial_\beta A_\gamma + \tfrac{1}{3}A_\alpha A_\beta A_\gamma\big) \qquad [30]$$

where K^μ is the Chern–Simons current,

$$\mathcal{P} = -\frac{1}{4\pi^2}\int dS_\mu K^\mu \qquad [31]$$

The integral [31] is over the base space boundary, S^3. The Chern–Pontryagin index of any gauge field configuration with finite (Euclidean) action (not only instantons) is quantized. This is because finite action requires $F_{\mu\nu}$ to vanish at large distances; equivalently, $A_\mu \to U^{-1}\partial_\mu U$. Using this in [30] renders [31] as

$$\mathcal{P} = \frac{1}{24\pi^2}\int dS_\mu\varepsilon^{\mu\alpha\beta\gamma} \times \mathrm{tr}(U^{-1}\partial_\alpha UU^{-1}\partial_\beta UU^{-1}\partial_\gamma U) \qquad [32]$$

which is the same as [20] and, for the same reason, is given by an integer $[\Pi^3(G) = Z]$. Alternatively, for instantons in the (Euclidean) Weyl gauge ($A_4 = 0$), which interpolate as x^4 passes from $-\infty$ to $+\infty$ between degenerate, classical vacua $A_i = 0$ and $A_i = -U^{-1}\nabla_i U$, $\mathcal{P}$ becomes

$$\begin{aligned}\mathcal{P} &= \frac{1}{4\pi^2}\int dx^4\, d^3x\,(\partial_4K^4 + \nabla\cdot\mathbf{K}) \\ &= \frac{1}{4\pi^2}\int d^3x\, K^4\,|_{x^4=\infty} \\ &= \frac{1}{24\pi^2}\int d^3x\,\varepsilon^{ijk}\,\mathrm{tr}(U^{-1}\partial_i UU^{-1}\partial_j UU^{-1}\partial U) \\ &= \omega(U)\end{aligned} \qquad [33]$$

We have assumed that the potentials decrease at large arguments sufficiently rapidly so that the gradient term in the first integrand does not contribute. This rederivation of [32] relies on the "motion" of an instanton between vacuum configurations of different winding numbers.

An explicit 1-instanton SU(2) solution ($\mathcal{P}=1$) is

$$A_\mu = \frac{-2\mathrm{i}}{(x-\xi)^2+\rho^2}\sigma_{\mu\nu}x^\nu \qquad [34]$$

(Upon reinserting the coupling constant g, which has been scaled to unity, the field profiles acquire the factor g^{-1}.) In [34], $\sigma_{\mu\nu} \equiv (1/4\mathrm{i})(\sigma^\dagger_\mu\sigma_\nu - \sigma^\dagger_\nu\sigma_\mu), \sigma_\mu \equiv (-\mathrm{i}\sigma, I)$. ξ is the "location" of the instanton, ρ is its "size," and there are three more implicit parameters fixing the gauge, for a total of eight parameters that are needed to specify a single SU(2) instanton. One can show that there exist N instanton/anti-instanton solutions ($\mathcal{P}=N/-N$) and in SU(2) they depend on $8N$ parameters. From [26] we see that at fixed N, instantons minimize the (Euclidean) action. Explicit formulas exist for the most general $N=2$ solution, while for $N \geq 3$ explicit formulas exhibit only $5N+7$ parameters. But algorithms have been found that construct the most general $8N$-parameter instantons. The 1-instanton solution is unchanged by SO(5) rotations, the maximal compact subgroup of the SO(5, 1) conformal invariance group for the Euclidean 4-space Yang–Mills equation [14a].

The Chern–Pontryagin index also appears in the Yang–Mills quantum action, for the following reason. Since all physical states respond to gauge transformations U_n with the universal phase $n\theta$ [24], physical states may be presented in factorized form,

$$\Psi(A) = \mathrm{e}^{\mathrm{i}\mu W(A)\theta}\Phi(A) \qquad [35]$$

where $\Phi(A)$ is invariant against all gauge transformations, small and large, while the phase response is carried by $W(A)$,

$$W(A^{U_n}) = W(A) + n \qquad [36]$$

An explicit expression for $W(A)$ is given by $-(1/4\pi^2)\int \mathrm{d}^3x\, K^0$, where K^0 is the time (fourth) component of K^μ, with dependence on the fourth variable suppressed, that is, K^0 is defined on 3-space,

$$W(A) = -\frac{1}{4\pi^2}\int \mathrm{d}^3x\, \varepsilon^{ijk}\,\mathrm{tr}\left(\tfrac{1}{2}A_i\partial_j A_k + \tfrac{1}{3}A_iA_jA_k\right) \qquad [37]$$

The gauge transformation properties of $W(A)$ are

$$\begin{aligned} W(A^U) &= W(A) + \frac{1}{8\pi^2}\int \mathrm{d}^3x\,\varepsilon^{ijk}\partial_i\,\mathrm{tr}(\partial_j UU^{-1}A_k) \\ &\quad + \frac{1}{24\pi^2}\int \mathrm{d}^3x\,\varepsilon^{ijk}\mathrm{tr}(U^{-1}\partial_i U\, U^{-1}\partial_j U\, U^{-1}\partial_k U) \end{aligned} \qquad [38]$$

The middle surface term does not contribute for well-behaved A; the last term is again $\omega(U)$, the winding number of the gauge transformation U. Thus, [36] is verified.

The universal gauge-varying phase $\mathrm{e}^{\mathrm{i}\theta W(A)}$, which multiplies all gauge-invariant functional states, may be removed at the expense of subtracting from the action

$$\theta\int \mathrm{d}^4x\,\partial_t W(A) = -\frac{\theta}{4\pi^2}\int \mathrm{d}^4x\,\partial_t K^0 = \theta\mathcal{P}$$

(as in [33]). Thus, the Yang–Mills quantum action extends [12] to

$$I_{\mathrm{YM}}{}^{\mathrm{quantum}} = \int \mathrm{d}^4x\,\mathrm{tr}\left(\frac{1}{2}F^{\mu\nu}F_{\mu\nu} + \frac{\theta}{16\pi^2}{}^*F^{\mu\nu}F_{\mu\nu}\right) \qquad [39]$$

The additional Chern–Pontryagin term in [35] does not contribute to equations of motion, but it is needed to render all physical states invariant against all gauge transformations, large and small. With this transformation, one sees that the θ-angle is a Lorentz invariant, but CP noninvariant effect. Evidently, specifying a classical gauge theory requires fixing a group; a quantized gauge theory is specified by a group and a θ-angle, which arises from topological properties of the gauge theory. The energy eigenvalues depend on θ, and distinct θ's correspond to distinct theories.

Note that the reasoning leading to [24] and [39] relies on exact quantum-mechanical arguments, while the instanton-based tunneling discussion is semiclassical.

Adding Fermions

When fermions couple to the gauge fields, the previously described topological effects are modified by action of the chiral anomaly. Dirac fields, either noninteracting but quantized, or unquantized but interacting with a gauge potential through a covariantly conserved current J^μ_a, $\mathcal{L}_\mathrm{I} = -J^\mu_a A^a_\mu$, also possess a chiral current $j^\mu_5 = \bar\psi\gamma^\mu\gamma_5\psi$, which satisfies

$$\partial_\mu j^\mu_5 = 2m\,\mathrm{i}\bar\psi\gamma_5\psi \qquad [40]$$

Here m is the mass, if any, of the fermions. j_5^μ is conserved for massless fermions, which therefore enjoy a chiral symmetry: $\psi \to e^{i\alpha\gamma_5}\psi$. However, when the interacting fermions are quantized, there arises correction to [40]; this is the chiral anomaly:

$$\partial_\mu \langle j_5^\mu \rangle_A = 2im\langle \bar{\psi}\gamma_5\psi\rangle_A + C\,{}^*F^{\mu\nu\,a}F^a_{\mu\nu} \quad [41]$$

C is determined by the fermion quantum numbers and coupling strengths. (For a single charged (e) fermion and a U(1) gauge potential, $C = e^2/8\pi^2$.) $\langle | \rangle_A$ signifies the fermionic vacuum matrix element in the presence of A_μ. The modified equation [41] indicates that even in the massless limit chiral symmetry remains broken due to the anomaly, which arises with quantized fermions.

$\langle j_5^\mu \rangle_A$ may also be presented as

$$\langle j_5^\mu \rangle_A = \mathrm{tr}\,\gamma_5\gamma^\mu \langle \psi\bar{\psi}\rangle_A \quad [42]$$

In Euclidean space $\langle \psi\bar{\psi}\rangle_A$ is the coincident-point limit of the resolvent $R(x,y;\mu)$ for the Dirac equation,

$$R(x,y;\mu) = \sum_\epsilon \frac{\psi_\epsilon(x)\,\psi_\epsilon^\dagger(y)}{\epsilon + i\mu} \quad [43]$$

Here ψ_ϵ is an eigenfunction of the massless, Euclidean Dirac operator in the presence of the gauge field A_μ,

$$i\gamma^\mu(\partial_\mu + A_\mu)\psi_\epsilon = \epsilon\psi_\epsilon \quad [44]$$

The coincident-point limit is singular, so R must be regulated: $R \to R - R_{\mathrm{Reg}}$ (we do not specify the regularization procedure). It then follows that

$$\begin{aligned}\partial_\mu\langle j_5^\mu\rangle &= 2i\mu\sum_\epsilon \frac{\psi_\epsilon^\dagger(x)\gamma_5\,\psi_\epsilon(x)}{\epsilon + i\mu} - \mathrm{tr}\,\gamma_5\,\gamma^\mu\partial_\mu R_{\mathrm{Reg}} \\ &= 2i\mu\sum_\epsilon \frac{\psi_\epsilon^\dagger(x)\gamma_5\psi_\epsilon(x)}{\epsilon + i\mu} + C\,{}^*F^{\mu\nu\,a}F^a_{\mu\nu}\end{aligned} \quad [45]$$

The first term on the right-hand side is the (Euclidean space) analog of the mass term in [40] or [41], while the second survives even after the regulators are removed, giving the anomaly $\mathrm{tr}\,{}^*F^{\mu\nu}F_{\mu\nu}$.

The anomaly formula [41], or more explicitly [45], is also the local form of the Atiyah–Singer index theorem, which follows after [45] is integrated over all space: The left-hand side integrates to zero. The integral of the first term on the right-hand side, $\int dx\,\psi_\epsilon^*\gamma_5\psi_\epsilon$, vanishes for $\epsilon \neq 0$ by orthogonality, because $\gamma_5\psi_\epsilon$ is an eigenfunction of [44] with eigenvalue $-\epsilon$. Only zero modes contribute to the ϵ sum since these can be chosen to be eigenfunctions of γ_5, $n_\pm$ of them satisfying $\psi_0 = \pm\gamma_5\psi_0$. For a single multiplet, the normalizations work out so that

$$n_+ - n_- = \frac{1}{16\pi^2}\int d^4x\,\mathrm{tr}\,{}^*F^{\mu\nu}F_{\mu\nu} \quad [46]$$

The result that the (signed) number of zero modes is the Chern–Pontryagin index is an instance of the Atiyah–Singer theorem. (In specific applications, one can frequently show that n_+ or n_- vanishes.) It, therefore, follows that in the background field of instantons, the Euclidean Dirac equation possesses zero modes.

Another viewpoint on the chiral anomaly arises within the functional integral formulation, where the exponentiated action is constructed from unquantized fields, over which the functional integration is performed. Here the classical action retains chiral symmetry $\psi \to e^{i\alpha\gamma_5}\psi$, but the Grassmann fermion measure $d\psi d\bar{\psi}$, once it is properly regularized, looses chiral invariance and acquires the anomaly,

$$d\psi d\bar{\psi} \to d\psi d\bar{\psi}\,\exp iC\int d^4x\,\alpha\mathrm{tr}\,{}^*F^{\mu\nu}F_{\mu\nu} \quad [47]$$

Evidently, the chiral anomaly involves the gauge-theoretic topological entity, the Chern–Pontryagin density. Not unexpectantly, the anomaly phenomenon affects significantly the topological properties of the gauge theory that are connected to $\mathcal{P}$ and were described previously.

When there is (at least) one massless fermion coupling to the Yang–Mills fields, the Yang–Mills θ-angle looses physical relevance. This is because a chiral transformation that redefines the massless Dirac field does not modify the classical action, but owing to the chiral noninvariance of the functional measure, [47], an anomaly term is induced in the (effective) quantum action. The strength of this induced term can be fixed so that it cancels the θ-term in [39]. Since field redefinition cannot affect physics, the elimination of the θ-term indicates that it had no physical relevance in the first place. In particular, energy eigenvalues no longer depend on θ.

An alternate argument for the same conclusion is based on the functional determinant that arises when the functional integral is performed over the massless Dirac field: $\det[\gamma^\mu(\partial_\mu + A_\mu)]$. The semiclassical tunneling analysis of the θ-angle is based on instantons, but in the presence of instantons the Dirac equation has a zero mode [46]. Consequently the determinant vanishes, tunneling is suppressed and so is the θ-angle.

However, in the standard model for particle physics, there are no massless fermions, so the presence of the θ-angle entails the following physical consequences. The tunneling amplitude Γ in leading semiclassical approximation is determined by the Euclidean action, namely the continuation of iI_{YM} in

[39] to imaginary time. This results in the same expression except that the topological θ-term acquires a factor of i. Only the 1-instanton and anti-instanton give the dominant contribution,

$$\Gamma \propto \cos\theta\, e^{-8\pi^2/g^2} \qquad [48]$$

where the coupling constraint g has been reinserted; the proportionality constant has not been computed, owing to infrared divergences. (Higher-instanton-number configurations contribute at an exponentially subdominant order and have thus far played no role in physics.) The tunneling leads to baryon decay, but fortunately at an exponentially small rate. More useful is the fact that instanton tunneling gives semiclassical evidence for the removal of an unwanted chiral U(1) Goldstone symmetry, which would be present in the standard model if the chiral anomaly did not interfere. Furthermore, the chiral anomaly facilitates the decay of the neutral pion to two photons; a process forbidden by other apparent chiral symmetries of the standard model, which in fact are modified by the chiral anomaly. Gauge fields in four dimensions must interact with anomaly free currents. This necessitates a precise adjustment of fermion content and charges so that the anomaly coefficients (analogs of "C" in [41]) vanish for currents coupled to gauge fields. Finally, θ provides a tantalizing source of CP violation in the strong-interaction sector of the standard model. But no experimental signal (e.g., neutron electric dipole moment) for this effect has been seen. At present, we do not know what mechanism is responsible for keeping θ vanishingly small.

These are the physical consequences of topological effects in four-dimensional gauge theories. Although they have provided experimentalists with only a few numbers to measure (e.g., $\pi^0 \to 2\gamma$ decay amplitude, prediction of anomaly-free arrangements of quarks and leptons in families), they have added enormously to our appreciation of the complexities of quantized gauge theories.

That chiral anomalies are an obstruction to consistent gauge interactions can be established within perturbation theory. A similar, but nonperturbative effect is seen in an SU(2) gauge theory with N Weyl fermion ($\gamma_5\psi = \pm\psi$) SU(2) doublets, which lead upon functional integration to $\det[\gamma^\mu(\partial_\mu + A_\mu)]^{N/2}$. But because $\Pi^4(\mathrm{SU}(2)) = Z_2$, there exists a single homotopy class of gauge transformations which are not deformable to the identity. One shows that the determinant changes sign when such a gauge transformation is performed. Thus, the theory is ill-defined for odd N. Consistent SU(2) gauge theories must possess an even number of Weyl fermion doublets, but such models have not found a place in physical theory.

Adding Bosons

Instantons are finite-action solutions to classical equations continued to imaginary time; they provide a semiclassical description of quantum-mechanical tunneling. A field theory may also possess finite-energy, time-independent (static) solutions to the real-time equations of motion. When these solutions are stable for topological reasons, they are called "solitons." Solitons give semiclassical evidence for the existence in the quantum field theory of a particle sector disjoint from the particles obtained by quantizing field fluctuations around the vacuum state. The soliton particles are heavy for weak coupling g. (Their energy is $O(1/g^2)$; the field profiles are $O(1/g)$.) They do not decay owing to the conservation of "charges" that do not arise from Noether's theorem but are topological.

Yang–Mills theory does not possess soliton solutions (except in five-dimensional spacetime, where the static solitons are just the four-dimensional instantons discussed previously). However, when a gauge theory, based on a simple group is coupled to a scalar field that undergoes symmetry breaking to U(1), soliton solutions exist. These are the 't Hooft–Polyakov magnetic monopoles, found in a SU(2) gauge theory with scalar fields in the adjoint representation, as well as various generalizations. The topological consideration that arises here concerns finite energy of the static, scalar field multiplet φ, which in the Weyl gauge is

$$E(\varphi) = \int d^3x \left(|(\boldsymbol{D}\varphi)^a \cdot (\boldsymbol{D}\varphi)^a|^2 + V(\varphi) \right) \qquad [49]$$

V is non-negative and possesses non trivial symmetry breaking zeroes. On the sphere S^2 at spatial infinity, φ must tend to such a zero. Thus, the fields belong to G/H, where G is the gauge group and H the unbroken subgroup. For the 't Hooft–Polyakov monopole these are SU(2) and U(1), respectively, and the scalar field provides a mapping of the sphere at infinity S^2 to $S^2 \approx \mathrm{SU}(2)/\mathrm{U}(1)$.

One now considers $\Pi^2(S^2) = \Pi^2(\mathrm{SU}(2)/\mathrm{U}(1)) = \Pi^1(\mathrm{U}(1)) = Z$, and one shows that the magnetic flux is determined by the winding number. Hence, the magnetic charge is quantized. Explicitly, the electromagnetic U(1) gauge field is given by

$$\begin{aligned} f_{\mu\nu} &\equiv \hat{\varphi}^a\, {}^*F^a_{\mu\nu} - \varepsilon_{abc}\hat{\varphi}^a (D_\mu\hat{\varphi})^b (D_\nu\hat{\varphi})^c \\ &= \partial_\mu a_\nu - \partial_\nu a_\mu \\ a_\mu &\equiv \hat{\varphi}^a A^a_\mu - \cos\alpha\,\partial_\mu\beta \end{aligned} \qquad [50]$$

where $\hat{\varphi}^a$ is the unit isovector, parametrized as $\hat{\varphi}^a = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)$. The manifestly conserved magnetic current

$$j^\mu_m = \partial_\nu {}^*f^{\mu\nu} \quad [51a]$$

is rearranged to read

$$j^\mu_m = -\tfrac{1}{2}\varepsilon^{\mu\alpha\beta\gamma}\varepsilon_{abc}\partial_\alpha\hat{\varphi}^a\partial_\beta\hat{\varphi}^b\partial_\gamma\hat{\varphi}^c \quad [51b]$$

and is nonvanishing because φ^a possesses zeroes, where $\partial_\alpha\hat{\varphi}^a$ acquires localized singularities. The magnetic charge

$$m = -\frac{1}{4\pi}\int \mathrm{d}^3x\, j^0_m = \frac{1}{4\pi}\int \mathrm{d}^3x\, \nabla\cdot \boldsymbol{b} \quad [52]$$

($b^i = \mathrm{U}(1)$ magnetic field: $-\frac{1}{2}\varepsilon^{ijk}f_{jk} = {}^*f^{i0}$) is given by the topological entity (Kronecker index of the mapping)

$$\begin{aligned} m &= \frac{1}{8\pi}\int \mathrm{d}^3x\, \varepsilon^{ijk}\varepsilon_{abc}\partial_i\hat{\varphi}^a\partial_j\hat{\varphi}^b\partial_k\hat{\varphi}^c \\ &= \frac{1}{8\pi}\int \mathrm{d}S^i\, \varepsilon^{ijk}\varepsilon_{abc}\hat{\varphi}^a\partial_j\hat{\varphi}^b\partial_k\hat{\varphi}^c \\ &= -\frac{1}{4\pi}\int \mathrm{d}S^i\, \varepsilon^{ijk}\partial_j\cos\alpha\,\partial_k\beta \end{aligned} \quad [53]$$

which readily evaluates the integer winding number.

The theory also supports charged magnetic monopole solutions called "dyons." Here the profiles involve time-periodic gauge potentials, where the time variation is just a gauge transformation $\partial_t A_\mu = D_\mu\lambda$. (Gauge-equivalent, static expressions have slow large-distance fall-off, which is removed by the time-dependent gauge function.) For dyons, the integer valued Chern–Pontryagin index, with the integration taken over all space and in time over the dyon period, reproduces the magnetic monopole strength.

Regrettably, these fascinating structures are not found in nature. Nor do they arise in the standard model, whose structure group is not simple, although speculative grand unified models, with simple G and $H = \mathrm{SU}(3)\times\mathrm{U}(1)$, would support magnetic monopoles and dyons. While challenged physically, the magnetic monopole phenomena have produced extensive and interesting mathematical analysis.

Gauge Theories in Two Dimensions

Two-dimensional gauge theories have only a few physical applications; edge states of the planar quantum Hall effect can be described by excitations moving on a line. However, the abelian model with fermions is useful in that it provides a very accurate reflection of topological behavior in the physically important four-dimensional theory.

Abelian Gauge Theory

Take the spatial interval to be $[-L, L]$. Homotopically nontrivial gauge transformations satisfy $\lambda(L) - \lambda(-L) = 2\pi n$ ($\Pi^1 U(1) = Z$). States $\Psi(A)$ of the free gauge theory that satisfy Gauss' law and respond with a θ-angle are

$$\begin{aligned} \Psi(A) &= \exp\frac{\mathrm{i}\theta}{2\pi}\int \mathrm{d}x\, A \\ \Psi(A+\partial\lambda) &= \mathrm{e}^{\mathrm{i}n\theta}\Psi(A) \end{aligned} \quad [54]$$

In this model, θ has the interpretation of a constant background electric field $\mathcal{E} = -\theta/2\pi$,

$$\begin{aligned} E\Psi(A) &= \mathcal{E}\Psi(A), \quad E \equiv F_{01} \\ \mathrm{i}\frac{\delta}{\delta A}\Psi(A) &= -\frac{\theta}{2\pi}\Psi(A) \end{aligned} \quad [55]$$

This also gives the energy eigenvalue:

$$\frac{1}{2}\int \mathrm{d}x\, E^2\Psi(A) = \frac{1}{2}\int \mathrm{d}x\, \mathcal{E}^2\Psi(A) \quad [56]$$

The phase may be removed by adding to the Lagrangian $-(\theta/2\pi)\int \mathrm{d}x\,\partial_t A$; equivalently, the action becomes

$$I^{\text{quantum}}_{\text{EM}} = \int \mathrm{d}^2x\left(-\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{\theta}{4\pi}\varepsilon^{\mu\nu}F_{\mu\nu}\right) \quad [57a]$$

which apart from a constant is also given by a formula with the background field:

$$I^{\text{quantum}}_{\text{EM}} = \frac{1}{2}\int \mathrm{d}x(E+\mathcal{E})^2 \quad [57b]$$

Because of gauge invariance, there is only one state, annihilated by E and carrying energy $\frac{1}{2}\int \mathrm{d}x\,\mathcal{E}^2$. Distinct θ (different $\mathcal{E}$) correspond to distinct theories.

We recognize in [57a] the two-dimensional Chern–Pontryagin density, contributing a total derivative to the action,

$$\mathcal{P} = \frac{1}{4\pi}\int \mathrm{d}^2x\, \varepsilon^{\mu\nu}F_{\mu\nu} \quad [58]$$

the Chern–Simons current, whose divergence is $\mathcal{P}$,

$$K^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu}A_\nu \quad [59]$$

and the Chern–Simons term, which carries the phase of Ψ

$$\int \mathrm{d}x\, K^0 = \frac{1}{2\pi}\int \mathrm{d}x\, A \quad [60]$$

For Euclidean-space gauge potentials, which are given at large distance by the pure gauge $2\pi n \tan^{-1} y/x$, $\mathcal{P}=n$. All this is just as in the four-dimensional theory, except there are no instantons and no tunneling.

Adding Fermions

The addition of massless fermions to the U(1) gauge theory results in the Schwinger model of massless quantum electrodynamics in two-dimensional spacetime. The equation of motion becomes

$$\partial_\mu F^{\mu\nu} = J^\nu \qquad [61]$$

with the vector current constructed from the Dirac fields as $J^\mu = \bar{\psi}\gamma^\mu\psi$. This current remains conserved in the quantized version because it couples to the gauge field. But the axial vector current $j_5^\mu = \bar{\psi}\gamma^\mu\gamma_5\psi$ acquires an anomaly that involves the Chern–Pontryagin density in [58],

$$\partial_\mu j_5^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu}F_{\mu\nu} \qquad [62]$$

The model is readily solved, and shows no θ-angle (background field) dependence in physical quantities. The solution is directly obtained by combining [61] with [62] into a second-order differential equation and using the matrix identity of two-dimensional Dirac (= Pauli) matrices: $\varepsilon^{\mu\nu}\gamma_\nu\gamma_5 = \gamma^\mu$. It follows that

$$\left(\Box + \frac{1}{\pi}\right)E = 0 \qquad [63]$$

So the theory describes a free massive photon (mass squared $= 1/\pi$ in units of $\hbar$ and the coupling constant, which have been scaled to unity), with no sign of a θ-angle (background field).

However, in parallel with four-dimensional behavior, the model with massive fermions regains a θ dependence in the particles' energy spectrum; a result that is established perturbatively, because a complete solution is not available.

Note that in the Schwinger model, the gauge particle ("photon") acquires a mass, even though local gauge invariance is preserved. This happens essentially for topological/anomaly reasons. Such topological mass generation is met again in three dimensions.

Adding Bosons

Scalar electrodynamics with a negative mass squared term in (3 + 1)-dimensional spacetime leads to the Higgs mechanism and short-range interactions due to the massive photons. In (1 + 1) spacetime dimensions, the model possesses instantons – scalar and gauge field profiles that solve the imaginary-time equations of motion – labeled by $\Pi^1(\mathrm{U}(1)) = Z$. These disorder the Higgs condensate so that the force between charged particles remains long-range, like in the positive mass-squared case. This is a vivid example of how excitations arising from nontrivial topological issues significantly effect physical content.

Gauge Theories in Three Dimensions

Gauge theories on three-dimensional spacetime, that is, evolving on a plane, have physical application to planar phenomena, like the quantum Hall effect. Also, the high-temperature limit of four-dimensional field theories is governed by the corresponding field theory in three Euclidean dimensions.

In three (more generally, odd) dimensions, there are no Chern–Pontryagin quantities, no Chern–Simon currents, no axial vector currents or anomalies (there is no γ_5 matrix). These are replaced by odd-dimensional entities that can modify Yang–Mills dynamics.

Yang–Mills and Other Gauge Theories

Using the three-index Levi-Civita tensor, one can construct a gauge-covariant, covariantly conserved vector, which can be added to the Yang–Mills equation. Thus, [14] can be modified to

$$D_\mu F^{\mu\nu} + \frac{m}{2}\varepsilon^{\mu\alpha\beta}F_{\alpha\beta} = J^\nu \qquad [64a]$$

or, equivalently, in terms of the dual-field strength ${}^*F^\mu \equiv \frac{1}{2}\varepsilon^{\mu\alpha\beta}F_{\alpha\beta}$,

$$\varepsilon^{\mu\nu\alpha}D_\mu {}^*F_\alpha + m{}^*F^\nu = J^\nu \qquad [64b]$$

For dimensional balance, m carries dimension of mass. Indeed, in the source-free case [64] implies

$$(D^\alpha D_\alpha + m^2){}^*F_\mu = \varepsilon_{\mu\alpha\beta}[{}^*F^\alpha, {}^*F^\beta] \qquad [65]$$

This shows that excitations are massive, even though local gauge invariance is preserved. Otherwise, as in the Dirac monopole case, the equations of motion are unexceptional.

However, for the quantum theory we need the action, whose variation produces the mass term in [64]. This is just the Chern–Simons term $W(A)$ in [37], multiplied by $-8\pi^2 m$ and now defined on (2 + 1)-dimensional spacetime:

$$I_{\mathrm{CS}} = 2m\int \mathrm{d}^3x\, \varepsilon^{\alpha\beta\gamma}\mathrm{tr}\left(\tfrac{1}{2}A_\alpha\partial_\beta A_\gamma + \tfrac{1}{3}A_\alpha A_\beta A_\gamma\right) \qquad [66]$$

Everything holds also in the abelian theory; the last term in [66] is then absent.

In this model, the mass is generated by a topological mechanism since I_{CS} possesses the usual attributes for a topological entity: it is diffeomorphisms invariant without a metric tensor; when the potentials are appropriately parametrized, it is given by a surface term. (In the abelian case, the appropriate parametrization is in terms of Clebsch decomposition, $A_\mu = \partial_\mu \theta + \alpha \partial_\mu \beta$.) Most importantly, in the nonabelian theory [66] changes by $8\pi^2 mn$ with three-dimensional gauge transformations carrying winding number n. Hence, for consistency of the nonabelian quantum theory, m must be quantized as $n/4\pi$ (in units of $\hbar$ and the coupling constant, which have been scaled to unity). All this is a clear field-theoretic analog to the quantum mechanics of the Dirac monopole, and just as for the magnetic monopole, a Hamiltonian argument for quantizing m can be constructed, as an alternative to the above action-based derivation.

The time component of [64] relates the electric and magnetic fields to the charge density:

$$\boldsymbol{D} \cdot \boldsymbol{E} - mB = \rho \qquad [67]$$

In the abelian case, the first term involves a total derivative and its spatial integral vanishes, leaving a formula that identifies magnetic flux with a total charge. At low energy, the mass term dominates the conventional kinetic term in [64], and the flux–charge relation becomes a local field-current identity,

$$m^* F^\nu \approx J^\nu \qquad [68]$$

These formulas have made Chern–Simons-modified gauge theories relevant to issues in condensed matter physics, for example, the quantum Hall effect. In the abelian case, m need not be quantized.

Adding Fermions

Three-dimensional Dirac matrices are minimally realized by 2×2 Pauli matrices. As a consequence, a mass term is not parity invariant; also, there is no γ_5 matrix, since the product of the three Dirac (= Pauli) matrices is proportional to I. While there are no chiral anomalies, there is the so-called parity anomaly: integrating a single doublet of massless SU(2) fermions one obtains $\Delta(\boldsymbol{A}) \equiv \det[\gamma^\mu(\mathrm{i}\partial_\mu + \boldsymbol{A}_\mu)]$, which should preserve parity and gauge invariance.

Since there are no anomalies in current divergences, $\Delta(\boldsymbol{A})$ is certainly invariant against infinitesimal gauge transformations. But for finite gauge transformations (categorized by $\Pi^3(\mathrm{SU}(2) = Z)$ one finds that $\Delta(\boldsymbol{A})$ is not invariant: when the gauge transformation belongs to an odd-numbered homotopy class, $\Delta(\boldsymbol{A})$ changes sign. To regain gauge invariance, one must either work with an even number of fermion doublets or, if only one doublet (more generally, odd number) is to be used, one must add to the gauge Lagrangian a parity-violating Chern–Simons term with half the correctly quantized coefficient, to neutralize the gauge non-invariance of $\Delta(\boldsymbol{A})$.

Alternatively, $\Delta(\boldsymbol{A})$ can be regularized in a gauge-invariant manner. But this requires massive, Pauli–Villars regulator fields, which produce a parity-violating expression for $\Delta(A)$. One cannot avoid the parity anomaly.

Adding Bosons

There are a variety of bosonic field models that one may consider: Abelian or nonabelian; with conventional kinetic term or supplemented by the Chern–Simons topological mass; or, for low energy, no kinetic term but only the Chern–Simons term, as in [68]. Abelian charged Bose fields in a Maxwell theory lead to vortex solitons, based on $\Pi^1(\mathrm{U}(1)) = Z$. These are just the instantons of the $(1+1)$-dimensional bosonic gauge theory discussed previously. With Maxwell kinematics there are no charged vortices, but these appear when the Chen–Simons mass is added; see [67]. Pure Chern–Simons kinematics, with no Maxwell term, can produce completely integrable soliton equations (Liouville, Toda) when the Bose field dynamics is appropriately chosen.

Conclusion

Topological effects in field theory are associated with the infinities and regularization that beset quantum field theories. These give rise to the chiral anomaly, parity anomaly (and scale symmetry anomalies, not discussed here). Yet the anomalies themselves are finite quantities that have topological significance (Atiyah–Singer, Chern–Pontryagin, Chern–Simons). This paradoxical pairing has not been understood. Nor can we explain why the anomalies interfere in a topological manner with symmetries associated with masslessness.

Although the range of topological effects in gauge theory is large, and even larger in non-gauge theories (sigma models, Skyrme models) the relevance to actual fundamental physics is confined to the θ-angle phenomenon, which is analyzed accurately and abstractly by reference to $\Pi^3(G)$ and to the interplay with fermions through the chiral anomaly. Instantons are relevant only to an approximate, semiclassical discussion. Although after much mathematical work, general instanton configurations are well understood, only the 1-instanton solution enjoys physical significance.

Other topological entities that fascinate are either nonexistent in fundamental physics or are relevant to

condensed matter physics (vortices, Chern–Simons effects). But here too, we note that the fundamental equation of condensed matter physics – the many-body Schrödinger equation – carries no evident topological structure. Only the phenomenological equations, which replace the fundamental one, give rise to topological intricacies.

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See also: Abelian and Nonabelian Gauge Theories Using Differential Forms; Abelian Higgs Vortices; Anomalies; BF Theories; Gauge Theories from Strings; Gauge Theory: Mathematical Applications; Quantum Field Theory: A Brief Introduction; Seiberg–Witten Theory.

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Normal Forms and Semiclassical Approximation

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Introduction

Quantum mechanics was born at the beginning of the twentieth century with the quantization rules for the harmonic oscillator and for the hydrogen atom. Such rules were almost immediately extended to more general systems by the so-called Bohr–Sommerfeld quantization rule: "the actions of the classical system can assume only those values which are integer multiples of $\hbar$." However, the actions are defined only in some special situations and, moreover, at the present time the Schrödinger equation is the paradigm of quantum mechanics. A question naturally arises: is there any relation between the eigenvalues of the Schrödinger operator and the numbers obtained by Bohr–Sommerfeld quantization rule (when available)?

According to common wisdom, the "Bohr–Sommerfeld numbers" are a first approximation to the eigenvalues of the Schrödinger operator in the so-called semiclassical limit. However, precise mathematical results on the subject were obtained only in the 1980s and a good understanding of the problem has been achieved only recently. In particular it is now clear how to compute higher-order corrections to the eigenvalues: this is done through suitable normal form procedures.

In the present article we will discuss the above questions for the case of perturbed harmonic oscillators, a case which, on the one hand, is physically relevant and, on the other, is well understood. We will only briefly discuss the quantization of perturbations of integrable systems.

A Statement

On $L^2(\mathbb{R}^n)$, consider the Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2}\Delta + V \qquad [1]$$

where Δ is the n-dimensional Laplacian and V is a smooth real potential having an absolute nondegenerate minimum at the origin. We are interested in

the eigenvalues of [1] close to zero. Introduce coordinates adapted to the normal modes, namely such that

$$V(x) = \sum_{i=1}^{n} \frac{\omega_i^2 x_i^2}{2} + O(\|x\|^3)$$

Assume

(H1) *Nonresonance*: There exist $\gamma > 0$ and $\tau \in \mathbb{R}$ such that, for any $k \in \mathbb{Z}^n - \{0\}$ one has

$$|\omega \cdot k| \geq \frac{\gamma}{|k|^\tau} \qquad [2]$$

(H2) $V(x) > 0$ for $x \neq 0$, and

$$\liminf_{|x| \to \infty} V(x) > 0$$

(H3) $V \in C^\infty(\mathbb{R}^n)$ and for any $r \geq 0$ there exists C_r such that

$$\left| \frac{\partial^{|\alpha|} V}{\partial x^\alpha}(x) \right| \leq C_{|\alpha|} \langle x \rangle^m, \quad \forall \alpha \in \mathbb{N}^n$$

where we used the notation $\langle x \rangle := (1 + \|x\|^2)^{1/2}$.

Theorem 1 *Assume that* (H1)–(H3) *hold. Then, for any positive* N, M *there exist positive constants* $\hbar_{N,M}, \epsilon_{N,M}, C^1_{N,M}, C^2_{N,M}$, *and a smooth function*

$$\mathcal{Z}_{N,M}(I_1, \ldots, I_n; \hbar)$$

such that, $\forall 0 < \epsilon \leq \epsilon_{N,M}$ *and* $0 < \hbar \leq \hbar_{N,M}\epsilon$, *the eigenvalues of* [1] *in* $[0, \epsilon)$ *have the representation*

$$\begin{aligned} \lambda_k = &\left(k + \tfrac{1}{2}\right) \cdot \omega\hbar + \mathcal{Z}_{N,M}\left(\left(k + \tfrac{1}{2}\right)\hbar; \hbar\right) \\ &+ R_{NM}(k, \hbar), \quad k \in \mathbb{N}^n, \ k_j \geq 1 \end{aligned} \qquad [3]$$

where

$$|R_{NM}(k, \hbar)| \leq C^1_{N,M}\epsilon^N + C^2_{N,M}\left(\frac{\hbar}{\epsilon}\right)^M$$

More precisely, for any $k \in \mathbb{N}^n$ *such that*

$$\left(k + \tfrac{1}{2}\right) \cdot \omega\hbar + \mathcal{Z}_{N,M}\left(\left(k + \tfrac{1}{2}\right)\hbar; \hbar\right) \in [0, \epsilon) \qquad [4]$$

there exists an eigenvalue $\lambda_k \in [0, \epsilon)$ *for which* [3] *holds, and vice versa, for any eigenvalue in* $[0, \epsilon)$ *there exists a k satisfying* [3] *and* [4]. *The function* $\mathcal{Z}_{N,M}(I_1, \ldots, I_n; 0)$ *coincides with the classical Birkhoff normal form of the system computed up to order N.*

The proof of the theorem is constructive, in the sense that it provides an algorithm allowing to construct explicitly, by elementary operations, the function $\mathcal{Z}_{N,M}$. One could choose $\epsilon = \epsilon(\hbar) = \hbar^\delta$ with some positive $\delta < 1$, obtaining a simpler statement valid for the eigenvalues in $[0, \hbar^\delta)$. It is also possible to weaken the nonresonance condition (H1) to the condition $\omega \cdot k \neq 0$ for $k \in \mathbb{Z}^n - \{0\}$.

A theorem very close to [1] was proved by Sjöstrand (1992) by a method different from the one that will be presented here (see also Graffi and Paul (1987)). In the analytic or Gevrey case (recall that a C^∞ function $f(x)$ is Gevrey in some domain if there exist constants C, σ such that, for all multi-indexes $\alpha \in \mathbb{N}^n$ one has

$$\left| \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \right| \leq C^{|\alpha|}(\alpha!)^\sigma$$

in the whole domain), the error can be reduced to be exponentially small with the parameters (Bambusi *et al.* 1999). Previous results dealing with compact perturbations of the harmonic oscillator were obtained by Bellissard and Vittot (1990). It is possible to deal also with the resonant case in which (H1) is violated. In this case the spectrum of the complete system is qualitatively different from the spectrum of the harmonic one. As discussed later, the normal form allows one to compute the main qualitative differences.

Birkhoff Normal Form

In this section we recall the procedure leading to classical Birkhoff normal form, whose quantization leads to the proof of Theorem 5.

Birkhoff's Theorem

The operator [1] is the quantization of the classical Hamiltonian

$$\sum_{i=1}^{n} \frac{\xi_i^2}{2} + V(x) \qquad [5]$$

Denote

$$H_0(\xi, x) := \sum_{j=1}^{n} \omega_j I_j, \quad I_j := \frac{\xi_j^2 + \omega_j^2 x_j^2}{2\omega_j} \qquad [6]$$

then we have

Theorem 2 *For any positive integer* $N \geq 2$ *there exist a neighborhood* $\mathcal{U}_N$ *of the origin and a canonical transformation* $\mathcal{T}_N : \mathbb{R}^{2n} \supset \mathcal{U}_N \to \mathbb{R}^{2n}$ *which puts the system* [5] *in Birkhoff normal form up to order N, namely such that*

$$H \circ \mathcal{T}_N = H_0 + Z^N + R_N \qquad [7]$$

where Z^N Poisson-commutes with H_0, namely $\{H_0; Z^N\} \equiv 0$ and R_N is small, that is,

$$|R_N(\xi, x)| \le C_N \|(\xi, x)\|^{N+1} \qquad [8]$$

Moreover, if the frequencies are nonresonant, namely

$$\omega \cdot k \neq 0, \quad \forall k \in \mathbb{Z}^n \backslash \{0\} \qquad [9]$$

the function Z^N depends on the actions I_j only. We recall that the Poisson bracket of two functions f and g is defined by

$$\{f; g\} := \sum_{j=1}^{n} \left(\frac{\partial f}{\partial \xi_j} \frac{\partial g}{\partial x_j} - \frac{\partial f}{\partial x_j} \frac{\partial g}{\partial \xi_j} \right) = -\{g; f\}$$

and coincides with the Lie derivative of g with respect to the Hamiltonian vector field of f.

Remark 1 In the case where the frequencies fulfill (H1) and the potential V is analytic (or of Gevrey class) the remainder can be reduced to be exponentially small with $\|(\xi, x)\|$.

Scheme of the Proof

Make the rescaling $\xi = \epsilon \xi'$, $x = \epsilon x'$. In terms of the primed variables, the Hamiltonian of the system [5] takes the form

$$H_\epsilon(\xi', x') = H_0(\xi', x') + \epsilon W(x') \qquad [10]$$

with

$$W(x') := \frac{V(\epsilon x') - \epsilon^2 \sum_{j=1}^{n} \omega_j^2 (x_j')^2/2}{\epsilon^3} = W_3(x') + \epsilon W_4(x') + \cdots \qquad [11]$$

and W_l is the Taylor polynomial of order l of V. In what follows we will omit primes from the scaled variables.

Given an auxiliary Hamiltonian χ_3, denote by Φ_t^3 the flow of the corresponding Hamiltonian vector field. We construct χ_3 so that $H_\epsilon \circ \Phi_\epsilon^3$ is in normal form up to order ϵ^2.

Remark 2 Given a C^∞ function g one has $g \circ \Phi_\epsilon^3 \sim \sum_{l=0}^{\infty} \epsilon^l g_l$, with

$$g_0 := g, \qquad g_l = \frac{1}{l}\{\chi_3; g_{l-1}\}, \quad l \ge 1 \qquad [12]$$

where $\sim$ denotes the fact that the left-hand side is asymptotic to the right-hand side (a precise definition appears later in the article). If both g and χ_3 are analytic then the series of $g \circ \Phi_\epsilon^3$ can be shown to converge in a neighborhood of the origin. Using [12] to compute $H_\epsilon \circ \Phi_\epsilon^3$, we get

$$H_\epsilon \circ \Phi_\epsilon^3 = H_0 + \epsilon[W_3 + \{\chi_3; H_0\}] + O(\epsilon^2)$$

So $H_\epsilon \circ \Phi_\epsilon^3$ is in normal form up to $O(\epsilon^2)$ provided χ_3 fulfills the so-called homological equation:

$$W_3 + \{\chi_3; H_0\} = Z_3 \qquad [13]$$

where the unknown function Z_3 has to be in normal form. Note that, since the operator

$$\chi \mapsto \{\chi; H_0\}$$

maps linearly polynomials of degree l into polynomials of degree l, eqn [13] can be interpreted as a linear equation in the finite-dimensional space of polynomials of degree 3 in the phase-space variables.

Lemma 1 *The homological equation* [13] *admits a solution* (χ_3, Z_3).

Proof Introduce the canonical coordinates (ζ, η) by

$$\zeta_j := \frac{1}{\sqrt{2}} \left(\frac{\xi_j}{\sqrt{\omega_j}} + \mathrm{i} x_j \sqrt{\omega_j} \right)$$
$$\eta_j := \frac{1}{\mathrm{i}\sqrt{2}} \left(\frac{\xi_j}{\sqrt{\omega_j}} - \mathrm{i} x_j \sqrt{\omega_j} \right) \qquad [14]$$

In these variables the unperturbed Hamiltonian H_0 reads $H_0 = \sum_{j \ge 1} \mathrm{i}\omega_j \zeta_j \eta_j$ and W_3 is transformed in a different polynomial, again of third order. The important fact is that in these coordinates the eigenvectors of the linear operator $\{H_0; .\}$ are the monomials

$$\zeta^k \eta^l \equiv \zeta_1^{k_1} \cdots \zeta_n^{k_n} \eta_1^{l_1} \cdots \eta_n^{l_n}$$

Indeed, one has $\{H_0; \zeta^k \eta^l\} = \mathrm{i}\omega \cdot (k - l) \zeta^k \eta^l$. As a consequence, writing

$$W_3(\zeta, \eta) = \sum_{k,l} C_{k,l} \zeta^k \eta^l$$

one can define the resonant set

$$\mathcal{R} := \{(k, l) \colon \omega \cdot (k - l) = 0\}$$

and

$$Z_3(\zeta, \eta) := \sum_{k,l \in \mathcal{R}} C_{k,l} \zeta^k \eta^l$$
$$\chi_3(\zeta, \eta) := \sum_{k,l \notin \mathcal{R}} \frac{C_{k,l}}{\mathrm{i}\omega \cdot (k - l)} \zeta^k \eta^l \qquad [15]$$

Going back to the original variables, one has the solution of the homological equation. □

Definition 1 The function Z_3 solving [13] will be called the resonant part of W_3 and will be denoted by $\langle W_3 \rangle$.

Using the function χ_3, one can transform the Hamiltonian to the form

$$H_0 + \epsilon Z_3 + \epsilon^2 R_3$$

Remark 3 Equation [12] allows to construct directly the Taylor expansion of R_3 in terms of the Taylor expansion of W and of its Poisson brackets with χ_3.

Iterating the construction (which however slightly changes due to the presence of Z_3), one gets the proof of Theorem 2.

Remark 4 In the nonresonant case $\omega \cdot (k - l) = 0$ implies that $k = l$; therefore, the resonant part of a polynomial is the sum of monomials of the form

$$\zeta^k \eta^k = I_1^{k_1} \cdots I_n^{k_n}$$

that is, it is a function of the actions only. Moreover, in this case one has $Z_3 = 0$, while in general $Z_4 \neq 0$.

Some Symbolic Calculus

To understand how to quantize the procedure of Birkhoff normal form, we consider the classical–quantum correspondence. It is well known that there are different procedures in order to associate an operator with a classical observable. Here we concentrate on the Weyl quantization rule.

To a function $f \in \mathcal{S}(\mathbb{R}^{2n})$ (Schwartz class), we associate an operator $\hat{f}$ acting on functions $\psi \in \mathcal{S}(\mathbb{R}^n)$, which is defined by

$$[\hat{f}\psi](x) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n \times \mathbb{R}^n} f\left(\frac{x+y}{2}, \xi\right) \times e^{\frac{i(x-y)\cdot\xi}{\hbar}} \psi(y)\, dy\, d\xi \qquad [16]$$

Definition 2 The operator [16] is called the Weyl quantization of f and in turn f is called the symbol of $\hat{f}$.

Using the method of oscillatory integrals, the Weyl quantization rule can be extended to much more general observables f. We recall that, roughly speaking, the method of oscillatory integrals consists in giving meaning to a formal expression of the form [16] by using successive integration by parts (see, e.g., Martinez (2001)).

Definition 3 A function $f \in C^\infty(\mathbb{R}^{2n})$ will be called a smooth symbol of class $S(\langle z \rangle^m)$ if, for any $r \geq 0$, there exists C_r such that

$$\left| \frac{\partial^{|\alpha|} f}{\partial z^\alpha}(z) \right| \leq C_{|\alpha|} \langle z \rangle^m, \quad \forall \alpha \in \mathbb{N}^{2n}$$

Where $\langle z \rangle$ is as defined earlier.

It is useful to extend such a definition to functions explicitly depending also on $\hbar$. This can be done in a straightforward way by asking the constants C_r to be independent of $\hbar$ in a neighborhood of the origin. Different classes of symbols can also be defined, but for our purpose this class is enough.

Theorem 3 *Let $f \in S(\langle z \rangle^m)$, $m \in \mathbb{R}$, and $\psi \in \mathcal{S}(\mathbb{R}^n)$; then the formal expression* [16] *is a well-defined oscillatory integral.*

Example 1 Under Weyl quantization rule, one has

$$\hat{\xi}_j = i\hbar \partial_{x_j}, \quad \hat{x}_j = x_j \quad \text{(multiplication operator)}$$
$$\widehat{\xi_j x_j} = \tfrac{1}{2}(\hat{\xi}_j \hat{x}_j + \hat{x}_j \hat{\xi}_j)$$

Definition 4 A sequence $(f_j)_{j \geq 0}$ with $f_j \in S(\langle z \rangle^m)$ will be called the asymptotic expansion of $f \in S(\langle z \rangle^m)$ if, for any integer N, there exist two positive constants $C_N, \hbar_N$ such that

$$f = \sum_{j=0}^{N} \hbar^j f_j + R_N$$

with $|R_N(z, \hbar)| \leq C_N \hbar^{N+1} \langle z \rangle^m$, and $\hbar \in (0, \hbar_N)$.

The key point for the quantization of the normal form procedure is the following.

Theorem 4 *Let $f \in S(\langle z \rangle^{m_1})$ and $g \in S(\langle z \rangle^{m_2})$; then there exists a unique $F \in S(\langle z \rangle^{m_1+m_2})$ such that*

$$\hat{F} = \hat{f}\hat{g} \quad \textit{(operator product!)}$$

moreover, one has

$$F = \exp\left(\frac{i\hbar}{2}(\partial_x \cdot \partial_\eta - \partial_y \cdot \partial_\xi)\right) \times (f(x, \xi) g(y, \eta))|_{y=x,\, \eta=\xi} \qquad [17]$$

Finally, F admits an asymptotic expansion in $\hbar$ which coincides with the formal expansion of [17].

The proof is obtained by using eqn [16] to write down an expression for $\hat{f}\hat{g}\psi$ and obtain a formula for F. Then, one shows that the formula is well defined and therefore the result is not formal.

Definition 5 In the above context, the symbol G of

$$\frac{i}{\hbar}\left[\hat{f}; \hat{g}\right] =: \hat{G}$$

will be called the "Moyal bracket" of f and g and will be denoted by $\{f; g\}_M$.

By formula [17], one has in particular

$$\{f; g\}_M = \{f; g\} + \hbar^2 \Delta_1(f, g) + O(\hbar^4) \qquad [18]$$

where

$$\Delta_1(f,g) = -\frac{1}{24}\left(\frac{\partial^3 f}{\partial\xi^3}\frac{\partial^3 g}{\partial x^3} - 3\frac{\partial^3 f}{\partial\xi^2\partial x}\frac{\partial^3 g}{\partial x^2\partial\xi} + 3\frac{\partial^3 f}{\partial\xi\partial x^2}\frac{\partial^3 g}{\partial x\partial\xi^2} - \frac{\partial^3 f}{\partial x^3}\frac{\partial^3 g}{\partial\xi^3}\right)$$

where we used a vector notation for the derivatives. If either f or g are polynomials of degree ≤ 2, then

$$\{f;g\}_{\mathrm{M}} = \{f;g\} \qquad [19]$$

Given a self-adjoint operator A and a smooth function $G:\mathbb{R}\to\mathbb{R}$, it is well known how to define by spectral theorem the operator $G(A)$. Suppose now that $A=\hat{f}$ for some symbol f. In general, one has $G(\hat{f}) \neq \widehat{G\circ f}$. However, by symbolic calculus (i.e., using eqn [17]), one has:

Lemma 2 *Denote* $I_j(x,\xi)=(\omega_j^2 x_j^2+\xi_j^2)/2\omega_j$. *Then, for any positive integer* k *there exists a function* $F_k(I_j,\hbar)$ *such that*

$$\widehat{(I_j)^k} = F_k(\hat{I}_j,\hbar)$$

where the right-hand side is defined by spectral calculus. Moreover, F_k *can be computed explicitly by the recursion formula* $F_{k+1}=I_jF_k+F_{k-1}\hbar^2(k^2-k+1)/4$.

As a consequence of this fact and of the fact that $[\hat{I}_j,\hat{I}_l]=0$, one has that the Weyl quantization of a polynomial function of the actions is a function of the action operators.

Semiclassical Normal Form

Let χ be a smooth symbol such that $\hat{\chi}$ is self-adjoint, and consider the group of unitary operators $X_\epsilon := \exp((\mathrm{i}\epsilon/\hbar)\hat{\chi})$. Let g be a smooth symbol; apply the unitary transformation X_ϵ to $\hat{g}$, namely compute $X_\epsilon\hat{g}X_\epsilon^{-1}$. Noting that (on a suitable domain)

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}(X_\epsilon\hat{g}X_\epsilon^{-1}) = X_\epsilon\frac{\mathrm{i}}{\hbar}[\hat{\chi};\hat{g}]X_\epsilon^{-1}$$

one has (formally!) the expansion of $X_\epsilon\hat{g}X_\epsilon^{-1}$ in ϵ:

$$X_\epsilon\hat{g}X_\epsilon^{-1} = \sum_{l\geq 0}\epsilon^l\widehat{g_{q,l}}$$

where

$$\widehat{g_{q,0}} := \hat{g}, \quad \widehat{g_{q,l}} = \frac{1}{l}\frac{\mathrm{i}}{\hbar}[\hat{\chi};\widehat{g_{q,l-1}}], \ l\geq 1 \qquad [20]$$

(Such a series can be interpreted as an asymptotic expansion provided one restricts the domain at each step of the approximation.) Equivalently, the symbol of $X_\epsilon\hat{g}X_\epsilon^{-1}$ is formally given by $\sum_l \epsilon_l g_{q,l}$ with

$$g_{q,0} := g, \quad g_{q,l} := \frac{1}{l}\{\chi; g_{q,l-1}\}_{\mathrm{M}}, \ l\geq 1 \qquad [21]$$

from which one sees a remarkable similitude with the classical equation. Moreover, [21] converges to [12] when $\hbar\to 0$.

Applying the unitary transformation generated by $\hat{\chi}$ to the Hamiltonian operator $\hat{H}_\epsilon$ (cf. eqn [10]), one has $X_\epsilon\hat{H}_\epsilon X_\epsilon^{-1} = \widehat{H_q^1}$ with

$$H_q^1 = H_0 + \epsilon[W_3 + \{\chi;H_0\}_{\mathrm{M}}] + O(\epsilon^2) \qquad [22]$$

$$\equiv H_0 + \epsilon[W_3 + \{\chi;H_0\}] + O(\epsilon^2) \qquad [23]$$

where we used the fact that H_0 is a quadratic polynomial, so that [19] holds. It is thus clear that Lemma 1 allows to solve also the quantum homological equation appearing in this context and to determine the symbol of the operator generating the unitary transformation putting the Hamiltonian operator in normal form up to corrections of order ϵ^2. Moreover, one can compute in terms of Moyal brackets (of polynomials!) the expansion of the symbol of the new remainder and of the normal form. Iterating the construction, one generates a well-defined semiclassical normal form of the quantum system.

Example 2 Denote by $Z_{q,l}, l=1,2\ldots,$ the term added to the semiclassical normal form at the lth step of the iterative construction. Explicitly, the first terms are given by

$$Z_{q,1} = \langle W_3\rangle = Z_3 \qquad [24]$$

$$Z_{q,2} = \langle W_4\rangle + \tfrac{1}{2}\langle\{\chi_3;W_3\}_{\mathrm{M}}\rangle + \tfrac{1}{2}\langle\{\chi_3;Z_3\}_{\mathrm{M}}\rangle \qquad [25]$$

$$Z_{q,3} = \langle W_5\rangle + \langle\{\chi_4;Z_3\}_{\mathrm{M}}\rangle + \tfrac{1}{3}\langle\{\chi_3;H_2\}_{\mathrm{M}}\rangle + \tfrac{1}{2}\langle\{\chi_3;W_{3,1}\}_{\mathrm{M}}\rangle + \langle\{\chi_3;W_4\}_{\mathrm{M}}\rangle \qquad [26]$$

where, according to Definition 1, $\langle\,.\,\rangle$ is the resonant part of its argument, χ_j is (formally) the symbol of the operator generating the jth unitary transformation, and

$$H_2 := \tfrac{1}{2}\{\chi_3;Z_3 - W_3\}_{\mathrm{M}}, \quad W_{3,1} := \{\chi_3;W_3\}_{\mathrm{M}}$$

Note that all the Moyal brackets involved contain polynomials of degree at most 4, so that they can be computed exactly using formula [18] which in this case does not contain corrections of order $\hbar^4$.

The problem in making previous construction rigorous is that all the series involved are in general

divergent. Moreover, it is not possible to show that the remainders appearing when truncating such series are small in a reasonable sense. Nevertheless, it is possible, using the tools of microlocal analysis, to show that the semiclassical normal form contains essentially all the information on the part of the spectrum close to zero.

The precise relation between the spectrum of the original Hamiltonian and the spectrum of the semiclassical normal form is captured by the following definition.

Let $H_1(\epsilon,\hbar), H_2(\epsilon,\hbar)$ be two families of self-adjoint operators; set $\mathrm{Spec}_\epsilon(H_{1,2}) := \mathrm{Spec}(H_{1,2}) \cap [0,\epsilon)$.

Definition 6 We say that

$$\mathrm{Spec}_\epsilon(H_1) = \mathrm{Spec}_\epsilon(H_2) \bmod (\epsilon^\infty + (\hbar/\epsilon)^\infty)$$

if for any $N, M > 0$ there exist $C^1_{N,M}$ and $C^2_{N,M}$ such that for any $\lambda_1 \in \mathrm{Spec}_\epsilon(H_1)$ there exists $\lambda_2 \in \mathrm{Spec}_\epsilon(H_2)$ such that $\lambda_1 = \lambda_2 + R_{N,M}$ with

$$|R_N| \le C^1_{N,M}\epsilon^N + C^2_{N,M}(\hbar/\epsilon)^M \qquad [27]$$

and conversely. Equation [27] has to hold for any couple $(\hbar,\epsilon)$ with ϵ and $(\hbar/\epsilon)$ small enough.

Theorem 5 *Assume* (H2) *and* (H3); *assume also*: (H1′) *There exist* $\gamma > 0$ *and* $\tau \in \mathbb{R}$ *such that, for any* $k \in \mathbb{Z}^n$, *one has*

$$\text{either } \omega\cdot k = 0 \quad \text{or } |\omega \cdot k| \ge \frac{\gamma}{|k|^\tau} \qquad [28]$$

Then there exists a polynomial function $\mathcal{Z}_q$ *such that one has*

$$\mathrm{Spec}_\epsilon(\hat{H}) = \mathrm{Spec}_\epsilon(\hat{H}_0 + \widehat{\mathcal{Z}_q}) \bmod \left(\epsilon^\infty + \left(\frac{\hbar}{\epsilon}\right)^\infty\right) \qquad [29]$$

The polynomial $\mathcal{Z}_q$ *coincides with the semiclassical normal form defined at the beginning of the section.*

Scheme of the proof It consists of six steps. (1) Make the unitary transformation $(U\psi)(x) := \epsilon^{n/4}\psi(\epsilon^{1/2}x)$ which transforms the Hamiltonian operator [1] into the Weyl quantized of $\epsilon H_\epsilon := \epsilon(H_0 + \epsilon^{1/2}W)$, but a Weyl quantization where $\hbar$ is substituted by $\hbar' := \hbar/\epsilon$. (2) Make a cutoff of H_ϵ, namely, fix R and consider a smooth function t such that $t(s) \equiv 1$ for $|s| \le R$, $t(s) \equiv 0$ for $|s| \ge 2R$, define $a(x,\xi) := W(x)t(\|(\xi,x)\|)$. (3) Compare the spectrum of the Hamiltonian $\hat{H}_\epsilon$ with the spectrum of $H^t := H_0 + \epsilon a$. By microlocal analysis, one has that, in any fixed bounded interval such spectra coincide modulo $\hbar^\infty$ (see, e.g., Martinez (2001)). (4) Rescale back the variables, namely apply the transformation U_ϵ^{-1} to H^t. (5) Apply the normal form algorithm to the so-obtained Hamiltonian showing that all the series involved are convergent in suitable norms. (6) Use again microlocal analysis to show that the spectrum of the semiclassical normal form coincides with the spectrum of the normalized operator with compactly supported symbol. □

Remark 5 Fix an arbitrary $1 > \delta > 0$ and link ϵ to $\hbar$ by $\epsilon := \hbar^\delta$. Then one obtains a simplified statement according to which the spectrum of [1] in $[0,\hbar^\delta]$ coincides modulo $\hbar^\infty$ with the spectrum of $\hat{H}_0 + \widehat{\mathcal{Z}_q}$ in the same interval.

Remark 6 In the case where the frequencies are nonresonant one has that the symbol of the normal form depends on the actions only. By Lemma 2 one has that also the quantization of the normal form is a function of the action operators only (explicitly computable), and therefore the spectrum of the normal form is given by a quantization formula as claimed in Theorem 1.

The Resonant Case

In the case where the frequencies are nonresonant, due to the particular structure of the normal form, one obtains a very precise information on the spectrum. In the case where there are some resonances, the situation is more difficult. In order to illustrate what happens we concentrate on the completely resonant case, that is, the case where all the frequencies are integer multiples of a single fundamental frequency ν.

In this case, the eigenvalues of $\hat{H}_0$ form a subset of $\mathbb{N}\hbar\nu + (1/2)|\omega|\hbar$ and are degenerate. One expects the nonlinear part to break such a degeneracy and to transform each eigenvalue in a small band. One can use the normal form to study the structure of the so-obtained band. To this end, the most relevant contribution is due to the first nonvanishing term of the normal form. For the sake of definiteness, we assume that this is the term of order 4, namely $\mathcal{Z}_4$. Denote

$$N := \mathcal{Z}_4\big|_{H_0^{-1}(1)}, \quad B(E) \equiv \left[E - \tfrac{1}{3}\nu\hbar, E + \tfrac{1}{3}\nu\hbar\right]$$

Theorem 6 *Fix* $1 > \gamma_1 > 1/2$, *then, provided* $\hbar$ *is small enough, one has*

$$\mathrm{Spec}(\hat{H}) \cap (\hbar, \hbar^{\gamma_1}) \subset \bigcup_{E \in \mathrm{Spec}(\hat{H}_0)} B(E) \qquad [30]$$

Moreover, denote by

$$E + \lambda_1(E,\hbar) \le \cdots \le E + \lambda_m(E,\hbar) \qquad [31]$$

the eigenvalues of $\hat{H}$ in $B(E)$ counted with multiplicity, then

$$\lambda_1(E, \hbar) = E^2 \mathrm{Min}\, N + E^2(O(\hbar/E) + O(E^{1/2})) \quad [32]$$

and similarly

$$E^2 \lambda_m(E, \hbar) = \mathrm{Max}\ N + E^2(O(\hbar/E) + O(E^{1/2})) \quad [33]$$

This statement is due to Bambusi, Charles, and Tagliaferro (see Bambusi 2004); for previous results, see Vũ Ngọc (1998).

Equation [30] shows that the spectrum has a band structure, while eqns [32] and [33] allow one to compute the minimum and the maximum of each band.

The idea of the proof is as follows. First forget high-order terms of the normal form, whose effect is included in the error terms. Then, due to the commutation property of the normal form with $\hat{H}_0$, one has that $\mathcal{Z}_4$ restricts to an operator acting on the eigenspaces of $\hat{H}_0$. On the classical side, one has that by Marsden–Weinstein procedure $\mathcal{Z}_4$ defines a classical Hamiltonian system on the manifold obtained by symplectic reduction of the original phase space. By the methods of geometric quantization, it turns out that the quantum operator acting on an eigenspace of $\hat{H}_0$ is a Toeplitz operator whose principal symbol is exactly the above reduced classical Hamiltonian. Then, the proof follows by classical properties of Toeplitz operators.

We point out that results of this kind are useful in the computation of the molecular spectra (Michel and Zhilinskii 2001, Zhilinskii 2001).

Quantization of KAM Tori

In this section we present a result on the quantization of KAM tori. It allows one to construct part of the spectrum of a close-to-integrable system.

We recall that a classical Hamiltonian system with n degrees of freedom is said to be integrable if it has n integrals of motion independent and in involution. If the energy surface is compact, then, by Arnol'd–Liouville theorem there exists a canonical transformation $\mathcal{T}_0 : \mathbb{R}^n \times \mathbb{T}^n \supset D \times \mathbb{T}^n \to \mathbb{R}^{2n}$ introducing action-angle variables, namely such that, denoting by K_0 the original integrable Hamiltonian, $K_0 \circ \mathcal{T}_0$ is independent of the angles $\phi \in \mathbb{T}^n$. Here, D is an open bounded domain.

Consider now a close-to-integrable analytic Hamiltonian system, namely a Hamiltonian system with Hamiltonian

$$K = K_0 + \epsilon K_1$$

where ϵ is a small parameter. We assume that, denoting again by $\mathcal{T}_0$ the canonical transformation introducing action-angle variables for the system K_0, one has that both $K_0 \circ \mathcal{T}_0$ and $K_1 \circ \mathcal{T}_0$ are real analytic on $D \times \mathbb{T}^n$. Then, the KAM theory applies. To state the corresponding result, denote by $D_0 \subset D$ a domain whose closure is contained in D.

Theorem 7 *Assume that $\forall I \in D$ one has*

$$\det\left(\frac{\partial^2 (K_0 \circ \mathcal{T}_0)}{\partial I^2}\right) \neq 0 \quad [34]$$

then there exists a positive constant ϵ_* and, for any ϵ with $|\epsilon| < \epsilon_*$, there exists a Gevrey canonical transformation $\mathcal{T}_\epsilon : D_0 \times \mathbb{T}^n \to \mathbb{R}^{2n}$ and a Cantor set $D_\epsilon \subset D_0$ with the following properties:

$$K \circ \mathcal{T}_\epsilon = Z(I) + R(I, \phi, \epsilon) \quad [35]$$

where $R(I, \phi, \epsilon)$ vanishes at infinite order on D_ϵ, that is, for any multi-index α there exists $C_{|\alpha|}$ such that one has

$$\left|\frac{\partial^{|\alpha|} R}{\partial (I, \phi)^\alpha}(I, \phi, \epsilon)\right| \leq C_{|\alpha|} \exp\left(-\frac{c}{|I - D_\epsilon|^\rho}\right) \quad [36]$$

with a suitable $\rho > 0$ and $|I - D_\epsilon|$ denoting the distance from D_ϵ. Moreover, as ϵ tends to zero, the measure of D_ϵ tends to the measure of D_0.

A particular consequence is that the set D_ϵ is foliated in invariant tori. From the proof, it also turns out that the motion on each torus is quasiperiodic with frequencies fulfilling the assumption (H1) stated earlier. Moreover, the tori are linearly stable and even more: they are stable in an exponential sense (namely, a solution starting $O(\mu)$ close to a torus takes at least a time $O(\exp(c/\mu^\rho))$ to double its distance from the torus).

Quantizing the normalizing transformation $\mathcal{T}_\epsilon$ by using the theory of Fourier integral operators, one can also put the quantum Hamiltonian in a suitable normal form which allows to deduce some spectral information on the system.

To fix ideas we restrict to the case where K is a natural system, namely it has the form (3.1), and is close to integrable in the above sense. Fix two parameters $E_1 < E_2$; assume (1) that $K^{-1}([-\infty, E_2 + \delta])$ is compact for some positive δ and (2) that the domain D_0 can be constructed in such a way that $\mathcal{T}_0 : D_0 \times \mathbb{T}^n \to K_0^{-1}([E_0, E_1])$ is a bijection and, moreover, the KAM condition [34] holds. Denote by $\theta \in \mathbb{Z}^n$ the Maslov class of the tori of K_0 (see, e.g., Lazutkin (1993)) and, having fixed some $0 < \sigma < 1$, define the set of indexes

$$\mathcal{I} := \{k \in \mathbb{Z}^n : |D_\epsilon - \hbar(k + \theta/4)| \leq \hbar^\sigma\} \quad [37]$$

Theorem 8 *There exist positive constants $\hbar_*$, c, C, and $\sigma < 1$, and a function $K_q : D_0 \times (0, \hbar_*) \to \mathbb{R}$ with the following property: for any $k \in \mathcal{I}$ there exists at least one eigenvalue of $\hat{K}$ in the interval*

$$\left[Z_q(\hbar(k+\theta/4),\hbar) - Ce^{-c/\hbar^\rho},\right.$$
$$\left.Z_q(\hbar(k+\theta/4),\hbar) + Ce^{-c/\hbar^\rho}\right] \quad [38]$$

One can also show that a large part of the spectrum is constructed in this way. This is obtained by comparing the semiclassical estimate of the number of eigenvalues in $[E_1, E_2]$ to the number of eigenvalues thus constructed.

Theorem 8 is due to Popov (2000); the quantization of KAM tori was initiated by Lazutkin and widely developed by Colin de Verdière, who obtained a result similar to Theorem 8 for the case where K is C^∞ and describes the geodesic flow on a compact Riemannian manifold (Colin de Verdière 1977).

See also: Central Manifolds, Normal Forms; $\hbar$-Pseudodifferential Operators and Applications; Optical Caustics; Quantum Mechanics: Foundations; Schrödinger Operators; Stationary Phase Approximation.

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N-Particle Quantum Scattering

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Introduction

The present article relies heavily on Quantum Mechanical Scattering Theory in this Encyclopedia and can be considered as its continuation. We use here freely the notation and results discussed in this article.

An important problem of scattering theory concerns the Schrödinger H operator of N, $N \geq 3$, interacting particles. Since the potential energy of pair interactions between particles depends on their relative positions only, it does not tend to zero at infinity in the configuration space of a system, even if the center-of-mass motion is removed. This is qualitatively different from the two-particle case. It turns out that asymptotically (for large times $t \to +\infty$ or $t \to -\infty$) an N-particle system splits up into clusters,

$$\mathcal{C}_1 \cup \cdots \cup \mathcal{C}_n = \{1, \ldots, N\}, \quad \mathcal{C}_k \cap \mathcal{C}_l = \emptyset \text{ if } k \neq l \quad [1]$$

Particles from the same cluster $\mathcal{C}_k$, $k = 1, \ldots, n$, form a bound state, and different clusters do not interact with each other. In particular, if $n = 1$ and $\mathcal{C}_1 = \{1, 2, \ldots, N\}$, then we have a bound state of the system. In another extreme case $n = N$, all particles are free. The asymptotic evolution determined by clusters $\mathcal{C}_1, \ldots, \mathcal{C}_n$ where $n \geq 2$, and bound states of all these clusters is called a scattering channel. Physically it is natural to expect that the list of all such channels is exhaustive, that is, no other scattering process is possible. This statement is called asymptotic completeness.

We emphasize that an N-particle system may be in different scattering states as $t \to +\infty$ and $t \to -\infty$ and different rearrangement processes are possible. For example, a three-particle system may asymptotically consist of free particles or a pair of particles may be in a bound state, whereas the third particle may be asymptotically free. If particles are free at both $-\infty$ and $+\infty$, then one speaks about elastic scattering; we have a capture if particles free at $-\infty$ form a bound state of a couple after the interaction; an opposite process, when a bound state at $-\infty$ gives three free particles, is known as a breakup. It is also possible that a bound state of one couple yields a bound state of

another pair (a rearrangement) or a bound state of a couple transforms into another bound state of the same couple (an excitation). All these processes are described by the scattering operator. On the contrary, if the whole system forms a bound state at $-\infty$ (i.e., $n=1$), then it remains in the same state for all t.

As far as monographic literature on N-particle scattering is concerned, we mention Dereziński and Gérard (1997), Faddeev (1965), Reed and Simon (1979), and Yafaev (2000).

Setting the Scattering Problem

Let us recall the definition of the N-particle Schrödinger operator (Hamiltonian)

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{V} \qquad [2]$$

If the configuration space of each particle is $\mathbb{R}^d$, then the operator $\mathbf{H}$ acts in the space $L_2(\mathbb{R}^{dN})$. The operator of kinetic energy (the "unperturbed" Hamiltonian) is

$$\mathbf{H}_0 = -\sum_{j=1}^{N}(2m_j)^{-1}\Delta_{x_j} \qquad [3]$$

where x_j and m_j are the position and mass of the particle labeled by j. The operator of potential energy of pair interactions of particles (the perturbation) $\mathbf{V}$ is the operator of multiplication by the function

$$V(x) = \sum_{i<j} V^{ij}(x_j - x_i), \quad i,j = 1,\ldots,N \qquad [4]$$

Set $\alpha=(ij)$, $x^\alpha = x_j - x_i$. It is assumed that the functions $V^\alpha(x^\alpha)$ tend to zero sufficiently rapidly as $|x^\alpha|\to\infty$ in $\mathbb{R}^d$. However, the function $V(x)\not\to 0$ as $|x|\to\infty$ in $\mathbb{R}^{dN}$ if at least one of the distances $|x_i - x_j|$ between particles remains bounded. This difficulty is manifest even for two particles ($N=2$), but in this case it disappears if the motion of the center of mass of the system is removed.

This means the following. Let the subspace X^{cm} of $\mathbb{R}^{dN}$ be distinguished by the condition

$$\sum_{j=1}^{N} m_j x_j = 0 \qquad [5]$$

and let X_{cm} be the orthogonal complement to X^{cm} in the space $\mathbb{R}^{dN}$ endowed with the scalar product

$$\langle x, y\rangle = 2\sum_{j=1}^{N} m_j \langle x_j, y_j\rangle_{\mathbb{R}^d} \qquad [6]$$

Then

$$L_2(\mathbb{R}^{dN}) = L_2(X_{\text{cm}}) \otimes L_2(X^{\text{cm}})$$

Denote by x_{cm}, x^{cm} the orthogonal projections of $x\in\mathbb{R}^{dN}$ on the subspaces X_{cm}, X^{cm}, respectively, so that $x=(x_{\text{cm}}, x^{\text{cm}})$. Clearly, the vector x_{cm} has components

$$x_{\text{cm}} = M^{-1}\sum_{j=1}^{N} m_j x_j, \quad M = \sum_{j=1}^{N} m_j$$

Let $T(p)$, $(T(p)f)(x_1,\ldots,x_N) = f(x_1+p,\ldots,x_N+p)$, be the operator of common translations of particles. The operator $\mathbf{H}$ commutes with $T(p)$, that is, $T(p)\mathbf{H} = \mathbf{H}T(p)$, for all $p\in\mathbb{R}^d$. It follows that

$$\mathbf{H} = K\otimes I + I\otimes H, \quad K = -(2M)^{-1}\Delta_{x_{\text{cm}}} \qquad [7]$$

where K is the kinetic energy operator of the center-of-mass motion.

The operator

$$H = H_0 + V \qquad [8]$$

acts in the space $\mathcal{H} = L_2(X^{\text{cm}})$. Here V is again the operator of multiplication by function [4]. The precise form of the differential operator H_0 depends on the choice of coordinates in X^{cm}. For example, if $N=2$ and $x=x_2-x_1$, then $H_0 = -(2m)^{-1}\Delta_x$ where $m = m_1 m_2 (m_1+m_2)^{-1}$. In the case $N=3$, a natural choice of coordinates in X^{cm} is given by one of the three sets of Jacobi variables:

$$x^{12} = x_2 - x_1$$

$$x_{12} = x_3 - (m_1+m_2)^{-1}(m_1x_1 + m_2x_2)$$

and similarly for x^{13}, x_{13} and x^{23}, x_{23}. In coordinates x^α, x_α the operator of kinetic energy is determined by the formula

$$H_0 = -(2m_\alpha)^{-1}\Delta_{x_\alpha} - (2m^\alpha)^{-1}\Delta_{x^\alpha}$$

where, for example,

$$(m^{12})^{-1} = m_1^{-1} + m_2^{-1}, \quad m_{12}^{-1} = (m_1+m_2)^{-1} + m_3^{-1}$$

If $N=2$, then $V(x)\to 0$ as $|x|\to\infty, x\in X^{\text{cm}}$, but this is no longer true for $N\geq 3$. According to eqn [7] the spectral and scattering theories for the operator $\mathbf{H}$ reduce to those for the operator H. However, for $N\geq 3$, this reduction is not really helpful.

Let us now consider a breakup $a=\{\mathcal{C}_1,\ldots,\mathcal{C}_n\}$ of an N-particle system into clusters $\mathcal{C}_1,\ldots,\mathcal{C}_n$, $1\leq n =: \#(a)\leq N$ satisfying conditions [1]. If interactions between different clusters are neglected, we obtain the operator

$$H_a = H_0 + V^a, \quad V^a = \sum_{l=1}^{n}\sum_{\alpha\in\mathcal{C}_l} V^\alpha \qquad [9]$$

In particular, $H_a = H_0$ if $\#(a)=N$ and $H_a = H$ if $\#(a)=1$. Let the operator of common translations

of particles from the same cluster be defined by the equation

$$(T_a(p_1,\ldots,p_n)f)(x_1,\ldots,x_N)=f(x'_1,\ldots,x'_N)$$

where $x'_j=x_j+p_l$ if $j\in\mathcal{C}_l$. The operator H_a commutes with the operators $T_a(p_1,\ldots,p_n)$ for all vectors $p_1,\ldots,p_n\in\mathbb{R}^d$. Let the subspace X^a be determined by the condition

$$\sum_{j\in\mathcal{C}_l} m_j x_j=0,\quad l=1,\ldots,n$$

and let X_a be the orthogonal complement to X^a in $X^{\rm cm}$ with respect to scalar product [6]. Clearly, $\dim X^a=(N-\#(a))d$, $\dim X_a=(\#(a)-1)d$. Then the space $\mathcal{H}$ splits into the tensor product

$$L_2(X^{\rm cm})=L_2(X_a)\otimes L_2(X^a) \qquad [10]$$

In what follows, x_a and x^a are the orthogonal projections of $x\in X^{\rm cm}$ on the subspaces X_a and X^a, respectively. The "external" variable $x_a=(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_n)$, where

$$\boldsymbol{x}_l=M_l^{-1}\sum_{j\in\mathcal{C}_l} m_j x_j,\quad M_l=\sum_{j\in\mathcal{C}_l} m_j$$

describes positions of centers of masses of the clusters. The "internal" variable x^a is the set of numbers $x_j-\boldsymbol{x}_l$ for all $j\in\mathcal{C}_l$ and all $l=1,\ldots,n$. Of course, for each l only $|\mathcal{C}_l|-1$ ($|\mathcal{C}_l|$ is the number of particles in a cluster $\mathcal{C}_l$) of variables $x_j-\boldsymbol{x}_l$ are independent. Set

$$K_a=-\Delta_{x_a}=-\sum_{l=1}^{n}(2M_l)^{-1}\Delta_{\boldsymbol{x}_l}$$

and

$$H^a=-\Delta_{x^a}+V^a$$

Then

$$H_a=K_a\otimes I+I\otimes H^a$$

Note that eigenvalues $\lambda^{a,n}$ of the operator H^a are sums over $l=1,\ldots,n$ of eigenvalues of the operators

$$H(\mathcal{C}_l)=H_0(\mathcal{C}_l)+\sum_{\alpha\in\mathcal{C}_l} V^\alpha$$

describing each cluster. Similarly, eigenfunctions $\psi^{a,n}$ of H^a are products of eigenfunctions of these operators. We usually write $\boldsymbol{a}$ instead of a couple $\{a,n\}$. In the following, the index $\boldsymbol{a}$ labels all cluster decompositions with $\#(a)\geq 2$. The eigenvalues $\lambda^{\boldsymbol{a}}$ of the operators H^a ($\lambda^a=0$ if $\#(a)=N$) are called thresholds of the Schrödinger operator [8]. If all functions $V^\alpha(x^\alpha)\to 0$ as $|x^\alpha|\to\infty$, then the essential spectrum of the operator H consists of the interval $[\lambda_0,\infty)$, where

$$\lambda_0=\min_{\boldsymbol{a}}\lambda^{\boldsymbol{a}}$$

(the Hunziker–Van Winter–Zhislin theorem). Moreover, the eigenvalues of the operator H may accumulate at its thresholds only.

The fundamental result of scattering theory for the N-particle Schrödinger operator can be formulated as follows. Let P^a be the orthogonal projection in $L_2(X^a)$ on the subspace $\mathcal{H}_a^{(p)}$ spanned by all eigenvectors $\psi^{a,n}$ of H^a, and let $\mathsf{P}_a=I\otimes\mathsf{P}^a$, where the tensor product is defined by eqn [10]. Then P_a commutes with the operator H_a. Set also $K_0=H_0$, $\mathsf{P}_0=I$. Suppose that for all α

$$|V^\alpha(x^\alpha)|\leq C(1+|x^\alpha|)^{-\rho},\quad \rho>1 \qquad [11]$$

(the short-range assumption). Then, for all a, the wave operators

$$W_a^\pm=W^\pm(H,H_a;\mathsf{P}_a)=\operatorname*{s-lim}_{t\to\pm\infty} e^{iHt}e^{-iH_at}\mathsf{P}_a$$

exist and are isometric on the ranges $\operatorname{Ran}\mathsf{P}_a$ of projections P_a. The subspaces $\operatorname{Ran}W_a^\pm$ are mutually orthogonal, and scattering is asymptotically complete:

$$\bigoplus_a \operatorname{Ran}W_a^\pm=\mathcal{H}^{(\rm ac)}$$

The singular continuous spectrum of H is empty, so the absolutely continuous subspace $\mathcal{H}^{(\rm ac)}$ of the operator H can be replaced by $\mathcal{H}\ominus\mathcal{H}^{(p)}$, where $\mathcal{H}^{(p)}$ is spanned by all eigenvectors of H.

These results can be reformulated in terms of scattering theory in a couple of spaces. Suppose that, for every a, eigenvectors $\psi^{a,n}$ are normalized and orthogonal if the corresponding eigenvalues $\lambda^{a,n}$ coincide. Let us introduce an auxiliary space

$$\hat{\mathcal{H}}=\bigoplus_{\boldsymbol{a}}\mathcal{H}_{\boldsymbol{a}},\quad \mathcal{H}_{\boldsymbol{a}}=\mathcal{H}_a=L_2(X_a) \qquad [12]$$

and an auxiliary operator

$$\hat{H}=\bigoplus_{\boldsymbol{a}} \boldsymbol{K}_{\boldsymbol{a}},\quad \boldsymbol{K}_{\boldsymbol{a}}=K_a+\lambda^{\boldsymbol{a}} \qquad [13]$$

in this space. Here and below, the sums are taken over all $\boldsymbol{a}$. We define an identification $\hat{J}:\hat{\mathcal{H}}\to\mathcal{H}$ by the relations

$$\hat{J}=\sum_{\boldsymbol{a}} J^{\boldsymbol{a}},\quad J^{\boldsymbol{a}}f_{\boldsymbol{a}}=f_{\boldsymbol{a}}\otimes\psi^{\boldsymbol{a}} \qquad [14]$$

where the tensor product is the same as in [10]. In particular, $J^0=I$. Since $H_aJ^{\boldsymbol{a}}=J^{\boldsymbol{a}}\boldsymbol{K}_{\boldsymbol{a}}$, the wave operators $W^\pm(H,\hat{H};\hat{J})$ exist and are isometric and complete, that is,

$$\operatorname{Ran}W^\pm(H,\hat{H};\hat{J})=\mathcal{H}^{(\rm ac)}$$

Thus, for states orthogonal to eigenvectors of H, evolution of an N-particle system decomposes

asymptotically into a sum of evolutions which are "free" in external variables x_a and are determined by eigenvalues and eigenfunctions of the Hamiltonians H^a in internal variables x^a. To be more precise, we have that, for all $f \in \mathcal{H}^{(ac)}$ and $t \to \pm\infty$,

$$\exp(-iHt)f = \sum_a \exp(-iK_a t) f_a^{\pm} \otimes \psi^a + o(1) \quad [15]$$

where

$$f_a^{\pm} = W^{\pm}(H, K_a; J^a)^* f$$

and the term $o(1)$ tends to zero in $\mathcal{H}$. The wave operator $W^{\pm}(H, K_a; J^a)$ describes the scattering channel where a system of N interacting particles splits up asymptotically (for $t \to \pm\infty$) into non-interacting clusters $\mathcal{C}_1, \ldots, \mathcal{C}_n$, $n \geq 2$, and particles from the same cluster $\mathcal{C}_l$ are in the bound state (if there are more than one particle in $\mathcal{C}_l$) given by the function $\psi^a(x^a)$. Somewhat loosely speaking, this implies that the continuous spectrum of the operator H consists of branches starting from all its thresholds.

Note that the scattering problem can equivalently be formulated without the separation of center-of-mass motion. In this case, a trivial decomposition with $\#(a) = 1$ should be added, and the set of thresholds of the operator $\boldsymbol{H}$ includes eigenvalues of the operator H.

The existence of the wave operators and their isometricity can be obtained by the Cook method. Only the asymptotic completeness is a difficult mathematical problem. It can be solved within the framework of the smooth method, which requires a study of boundary values of resolvents as the spectral parameter z approaches the continuous spectrum or, equivalently, a study of a large-time behavior of evolution operators.

The scattering operator

$$S = W^+(H, \hat{H}; \hat{J})^* W^-(H, \hat{H}; \hat{J})$$

is unitary on the space $\hat{\mathcal{H}}$ and commutes with the operator $\hat{H}$. Its component $S_{ab} : \mathcal{H}_b \to \mathcal{H}_a$ describes a process where a system in a state $\boldsymbol{b}$ as $t \to -\infty$ goes over in a state $\boldsymbol{a}$ as $t \to +\infty$. Diagonalizing the operator $\hat{H}$ by a unitary operator $\hat{F}, (\hat{F}\hat{H}f)(\lambda) = \lambda(\hat{F}f)(\lambda), \lambda > \lambda_0$, we obtain the scattering matrix $S(\lambda)$ defined by the equation $(\hat{F}Sf)(\lambda) = S(\lambda)(\hat{F}f)(\lambda)$. In its turn, the scattering matrix is also a matrix operator with components $S_{ab}(\lambda)$. For $N \geq 3$, the structure of the scattering matrix is essentially more complicated than for $N = 2$. This is discussed in some detail in the next section.

Resolvent Equations for Three-Particle Systems

Let the Hamiltonian $\boldsymbol{H}$ be defined by eqns [2]–[4], where $N = 3$, and let the configuration space of each particle be $\mathbb{R}^d$, $d \geq 3$. The operator H acts in the space $\mathcal{H} = L_2(X^{cm})$, where the subspace $X^{cm} \subset \mathbb{R}^{3d}$ is distinguished by condition [5]. Let $R_0(z) = (H_0 - z)^{-1}, R(z) = (H - z)^{-1}$. Since $V(x)$ does not tend to 0 as $|x| \to \infty, x \in X^{cm}$, in the three-particle case, the resolvent equation

$$R(z) = R_0(z) - R_0(z) V R(z) \quad [16]$$

is not Fredholm even for $\operatorname{Im} z \neq 0$.

To overcome this difficulty, Faddeev (1965) derived a system of equations for components of the resolvent. The entries of this system are constructed in terms of three Hamiltonians

$$H_\alpha = H_0 + V^\alpha$$

$\alpha = (12), (13), (23)$, containing only one pair interaction each, and their resolvents $R_\alpha(z) = (H_\alpha - z)^{-1}$. Let us write down the resolvent equation for each pair H_α, H

$$R(z) = R_\alpha(z) - R_\alpha(z) \sum_{\beta \neq \alpha} V^\beta R(z)$$

We multiply it by $|V^\alpha|^{1/2}$ and set

$$\boldsymbol{r}_\alpha^0(z) = |V^\alpha|^{1/2} R_\alpha(z), \quad \boldsymbol{r}_\alpha(z) = |V^\alpha|^{1/2} R(z)$$
$$\boldsymbol{t}_{\alpha,\alpha}(z) = 0, \quad \boldsymbol{t}_{\alpha,\beta}(z) = |V^\alpha|^{1/2} R_\alpha(z) (V^\beta)^{1/2}$$

where $(V^\beta)^{1/2} = V^\beta |V^\beta|^{-1/2}$. This yields a system of equations

$$\boldsymbol{r}_\alpha(z) = \boldsymbol{r}_\alpha^0(z) - \sum_{\beta \neq \alpha} \boldsymbol{t}_{\alpha,\beta}(z) \boldsymbol{r}_\beta(z) \quad [17]$$

for the operators $\boldsymbol{r}_\alpha(z)$. Note that the resolvent $R(z)$ can be recovered from its components $\boldsymbol{r}_\alpha(z)$ by the formula

$$R(z) = R_0(z) - R_0(z) \sum_\alpha (V^\alpha)^{1/2} \boldsymbol{r}_\alpha(z)$$

It is convenient to rewrite eqn [17] in the matrix notation

$$\boldsymbol{r}(z) = \boldsymbol{r}^0(z) - \boldsymbol{t}(z) \boldsymbol{r}(z) \quad [18]$$

where $\boldsymbol{r}^0(z) = \{\boldsymbol{r}_\alpha^0(z)\}, \boldsymbol{r}(z) = \{\boldsymbol{r}_\alpha(z)\}$ are the "vector" operators in the three-component space $L_2^{(3)}(X^{cm})$ and $\boldsymbol{t}(z) = \{\boldsymbol{t}_{\alpha,\beta}(z)\}$ is the "matrix" operator in this space.

The advantage of eqn [17] compared to [16] is that the operators $\boldsymbol{t}_{\alpha,\beta}(z)$ are compact for $\operatorname{Im} z \neq 0$. This can be deduced from the fact that the product $V^\alpha(x^\alpha) V^\beta(x^\beta)$, where $\alpha \neq \beta$ tends to 0 as

$|x| \to \infty, x \in X^{\mathrm{cm}}$, provided that $V^\alpha(x^\alpha) \to 0$ as $|x^\alpha| \to \infty$ for all α. Moreover, the homogeneous equation [17] has only a trivial solution. Indeed, if for some z with $\operatorname{Im} z \neq 0$

$$f_\alpha = -\sum_{\beta \neq \alpha} \boldsymbol{t}_{\alpha,\beta}(z) f_\beta \qquad [19]$$

then the function

$$u = \sum_\alpha (V^\alpha)^{1/2} f_\alpha$$

satisfies the equation $u = -R_0(z)Vu$. Since the operator H is self-adjoint, this implies that $u = 0$ and hence $f_\alpha = 0$ for all α. According to the Fredholm alternative, eqns [17] for $\boldsymbol{r}_\alpha(z)$ or [18] for $\boldsymbol{r}(z)$ can be solved if $\operatorname{Im} z \neq 0$, that is,

$$\boldsymbol{r}(z) = (I + \boldsymbol{t}(z))^{-1} \boldsymbol{r}^0(z) \qquad [20]$$

This equation allows one to deduce the existence of necessary boundary values of the "sandwiched" resolvent $R(z)$ from similar results for the resolvents $R_\alpha(z)$ of the "two-particle" operators H_α. In its turn, $R_\alpha(z)$ can be expressed in terms of the resolvent $R^\alpha(z)$ of the operator H^α acting in the space $L_2(\mathbb{R}^d)$. Indeed, in the "mixed" representation (ξ_α, x^α), where the Fourier transform in the variable x_α is performed and the variable ξ_α is dual to x_α, we have

$$(R_\alpha(z)f)(\xi_\alpha, x^\alpha) = (R^\alpha(z - (2m_\alpha)^{-1}|\xi_\alpha|^2)f) \times (\xi_\alpha, x^\alpha) \qquad [21]$$

The passage to the limit $\operatorname{Im} z \to 0$ requires that assumption [11] be satisfied for $\rho > 2$. Moreover, we have to suppose that the operators H^α do not have the so-called zero-energy resonances as well as eigenvalues embedded in the continuous spectrum. Then the operator functions $\langle x^\alpha \rangle^{-l} R^\alpha(z) \langle x^\alpha \rangle^{-l}, l > 1$, $\langle x^\alpha \rangle = (1 + |x^\alpha|^2)^{1/2}$, are analytic in the complex plane cut along $[0, \infty)$, they have poles only at the points $\lambda^{\alpha,n}$, and are continuous up to the cut, the point $z = 0$ included. In particular, it follows from eqn [21] that, if the operators H^α do not have negative eigenvalues, then the operator functions $\langle x^\alpha \rangle^{-l} R_\alpha(z) \langle x^\alpha \rangle^{-l}, l > 1$, are also analytic in the complex plane cut along $[0, \infty)$ and are continuous up to the cut.

The next result is of genuinely three-particle nature and is crucial for the study of the operator $\boldsymbol{t}(z)$. The operator functions $\langle x^\alpha \rangle^{-l} R_0(z) \langle x^\beta \rangle^{-l}, \alpha \neq \beta, l > 1$, are continuous in norm up to the cut along $[0, \infty)$.

Now it follows from eqn [20] that the operator-valued functions $\boldsymbol{r}_\alpha(z)|V^\alpha|^{1/2}$ are continuous up to the cut $(0, \infty)$ except points $\lambda \in (0, \infty)$, where the homogeneous equation [19] for $z = \lambda \pm \mathrm{i}0$ has a nontrivial solution. The set $\mathcal{N} = \mathcal{N}_+ \cup \mathcal{N}_-$ of such points $\lambda \in (0, \infty)$ is closed and has Lebesgue measure zero. In particular, the operators $\langle x^\alpha \rangle^{-l}, l > 1$, are H-smooth on any compact subinterval of $\Lambda = (0, \infty) \setminus \mathcal{N}$. Therefore, the smooth method of scattering theory can be directly applied. It yields the existence and completeness of the wave operators $W_\pm(H, H_0)$. In this case, three-particles are necessarily asymptotically free.

"Two-particle" channels of scattering arise if the operators H^α have negative eigenvalues. To simplify notation, we assume that every H^α has exactly one eigenvalue $\lambda^\alpha < 0$. Moreover, it is supposed that the corresponding eigenfunction $\psi^\alpha(x^\alpha)$ tends to zero sufficiently rapidly as $|x^\alpha| \to \infty$. Analytically, the appearance of new channels is due to new singularities of the resolvents. Indeed, in this case

$$R^\alpha(z) = (\lambda^\alpha - z)^{-1} P^\alpha + \hat{R}^\alpha(z)$$

where the function $\hat{R}^\alpha(z)$ is analytic and continuous up to the cut in the complex plane cut along $[0, \infty)$. It follows from eqn [21] that in this case the resolvent $R_\alpha(z)$ contains the additional term

$$((2m_\alpha)^{-1}|\xi_\alpha|^2 + \lambda^\alpha - z)^{-1} \otimes P^\alpha$$

which is analytic only in the complex plane cut along $[\lambda^\alpha, \infty)$. To take these terms into account, system [17] should be further rearranged. This yields the following result. Let us set

$$\mathsf{G}_{\alpha 0} = \langle x^\alpha \rangle^{-l}(I - P_\alpha), \quad \mathsf{G}_{\alpha 1} = \langle x_\alpha \rangle^{l} (J^\alpha)^* \sum_{\beta \neq \alpha} V^\beta \qquad [22]$$

Then, for all $\alpha, \beta, i, j = 0, 1$, a suitable $l > 1$ and $\lambda_0 = \min\{\lambda^\alpha\}$, the operator functions $\mathsf{G}_{\alpha i} R(z) \mathsf{G}^*_{\beta j}$ are norm continuous as z approaches the cut (λ_0, ∞) at the points of $\Lambda = (\lambda_0, \infty) \setminus \mathcal{N}$, where $\mathcal{N}$ is again a closed set of measure zero. In particular, the operators $\mathsf{G}_{\alpha 0}$ and $\mathsf{G}_{\alpha 1}$ are H-smooth on any compact subinterval of Λ.

In the multichannel case, to fit scattering for the Hamiltonian H into the framework of smooth theory, it is convenient to reformulate the result in terms of scattering theory in a couple of spaces. Let the space $\hat{\mathcal{H}}$, the operator $\hat{H}$, and the identification $\hat{J}$ be defined by eqns [12], [13], and [14], respectively, where the index $\boldsymbol{a}$ takes four values $\boldsymbol{a} = 0, \alpha$ and $\alpha = (12), (13), (23)$. One, further, needs to introduce auxiliary identifications

$$J^0 = I - \sum_\alpha P_\alpha$$

and

$$\hat{J} = J^0 \oplus \bigoplus_\alpha J^\alpha$$

The H- (and $\hat{H}$-) smoothness of operators [22] imply that the wave operators

$$W^{\pm}(H,\hat{H};\hat{J}) \quad \text{and} \quad W^{\pm}(\hat{H},H;\hat{J}^*)$$

exist.

The operators $W^{\pm}(H,\hat{H};\hat{J})$ are isometric because

$$\operatorname*{s-lim}_{|t|\to\infty} P_\alpha \exp(-\mathrm{i}H_0 t) = 0 \qquad [23]$$

and the operators $P_\alpha P_\beta$ are compact for $\alpha \neq \beta$. Using that the operator

$$\hat{J}\hat{J}^* - I = \sum_{\alpha\neq\beta} P_\alpha P_\beta$$

is compact (whereas $\hat{J}\hat{J}^* - I$ is not), we see that the operators $W^{\pm}(\hat{H},H;\hat{J}^*)$ are also isometric. Finally, we remark that, by eqn [23],

$$W^{\pm}(H,\hat{H};\hat{J}) = W^{\pm}(H,\hat{H},\hat{J})$$

This implies the asymptotic completeness.

Let us discuss properties of the scattering matrix in the one-channel case where the pair operators H^α do not have negative eigenvalues. The scattering matrix $S(\lambda): L_2(\mathbb{S}^{2d-1}) \to L_2(\mathbb{S}^{2d-1})$, $\lambda > 0$, is of course a unitary operator, but in contrast to the two-particle case the operator $S(\lambda) - I$ is not compact because its kernel contains the Dirac functions $\delta(\xi_\alpha - \xi'_\alpha)$. Nevertheless, the structure of its singularities can be explicitly described. Actually, let $S_\alpha(\lambda)$ be the "two-particle" scattering matrix for the pair H_0, H_α. Then

$$S(\lambda) = S_{12}(\lambda)S_{23}(\lambda)S_{13}(\lambda)\tilde{S}(\lambda)$$

where the operator $\tilde{S}(\lambda) - I$ is compact.

The approach described briefly in this section relies on a kind of an advanced perturbation theory where the free problem is determined by the set of all sub-Hamiltonians. Its generalization to the case of an arbitrary number of particles meets with numerous difficulties. A different, nonperturbative, approach which works well for any number of particles will be discussed in the next section.

A purely time-dependent method in three-particle scattering is exposed in Enss (1983).

Nonperturbative Approach

Now N and d are arbitrary. In the nonperturbative approach (see Graf (1990), Sigal and Soffer (1989), and Yafaev (1993)) the operators H and H_0 as well as the Hamiltonians of all subsystems are treated on an equal basis. It is supposed that all pair potentials satisfy condition [11]. No assumptions on subsystems are required.

The starting point of this approach is the limiting-absorption principle, which claims that the operator $\langle x\rangle^{-l}$, $x \in X^{\mathrm{cm}}$, for $l > 1/2$ is H-smooth on any compact interval Λ not containing the thresholds and eigenvalues of H. Its proof relies on the Mourre commutator method (see Cycon *et al.* (1987)). To be more precise, it is deduced from the following estimate:

$$\mathrm{i}([H,A]f,f) \geq c\|f\|^2, \quad c = c(\lambda) > 0$$
$$f \in E(\Lambda_\lambda)\mathcal{H} \qquad [24]$$

for the commutator of H with the generator of translations

$$A = -\mathrm{i}\sum_j (x_j\partial_j + \partial_j x_j)$$

Here x_j are coordinates of $x \in X^{\mathrm{cm}}$ in some orthonormal (with respect to scalar product [6]) basis in X^{cm}, λ is neither a threshold nor an eigenvalue of the operator H and Λ_λ is a sufficiently small interval. Very roughly speaking, the Mourre estimate [24] means that, similarly to the two-particle case, the observable

$$(A\mathrm{e}^{-\mathrm{i}Ht}f, \mathrm{e}^{-\mathrm{i}Ht}f)$$

is a strictly increasing function of t for all $f \in \mathcal{H}^{(\mathrm{ac})}$.

The limiting-absorption principle implies that the singular continuous spectrum of the operator H is empty, but it is not sufficient for scattering theory. If the limiting-absorption principle were true for the critical value $l = 1/2$, then it would imply asymptotic completeness. Unfortunately, the operator $\langle x\rangle^{-1/2}$ is definitely not smooth even with respect to the free operator H_0. However, by introducing an auxiliary differential operator we can fix this problem. This leads to the radiation estimates. These estimates look differently in different regions of the configuration space. Choose any cluster decomposition $a = (\mathcal{C}_1, \ldots, \mathcal{C}_n)$. The radiation estimate morally implies that the motion of a system is asymptotically free in the variable x_a (describing the relative motion of clusters) in the region where particles from each cluster $\mathcal{C}_l$, $l = 1, \ldots, n$, are close to each other compared to distances between different clusters. On the contrary, this motion is very complicated in the variable x^a pertaining to bound states of different clusters. In particular, the radiation estimate is the same as for the two-particle case in the "free" region where all particles are far from each other.

To be more precise, let $\nabla_a = \nabla_{x_a}$ be the gradient in the variable x_a and let $\nabla_a^\perp$,

$$(\nabla_a^\perp u)(x) = (\nabla_a u)(x) - |x_a|^{-2}\langle(\nabla_a u)(x), x_a\rangle x_a$$

be its orthogonal projection in X_a on the subspace orthogonal to the vector x_a. Let χ_a be the

characteristic function of a closed cone $Y_a \subset X^{\mathrm{cm}}$ satisfying the condition $Y_a \cap X_b = \emptyset$ for all b such that $X_a \not\subset X_b$. Then the operator

$$G_a = \chi_a \langle x \rangle^{-1/2} \nabla_a^{\perp}$$

is H-smooth on Λ.

A proof of the radiation estimates is based on the consideration of the commutator of H with some differential operator $M = -\mathrm{i} \sum (m^{(j)} \partial_j + \partial_j m^{(j)})$, where $m^{(j)} = \partial m / \partial x_j$. Here m (it depends on a) is a specially constructed function satisfying the following properties:

1. $m(x)$ is homogeneous (for $|x| \geq 1$) of order 1;
2. for any b it does not depend on x^b in some conical neighborhood of the subspace X_b;
3. $m(x)$ is convex; and
4. $m(x) = \mu_a |x_a|, \mu_a \geq 1$, on support of the function χ_a.

Note that we can set $m(x) = |x|$ in the case of the operator H_0.

Due to properties (1) and (2) the commutator $[V, M]$ is a short-range function (estimated by $\langle x \rangle^{-1-\varepsilon}$ for $\varepsilon > 0$). Due to properties (3) and (4) the commutator $[H_0, M] \geq c G_a^* G_a, c > 0$, up to short-range terms. The estimate

$$[H, M] \geq c G_a^* G_a - c_1 \langle x \rangle^{-1-\varepsilon}$$

implies that the operator G_a is H-smooth on Λ.

The main difficulty in the N-particle problem is that pair potentials $V^{\alpha}(x^{\alpha})$ do not tend to zero as $|x| \to \infty$. The idea of the proof of asymptotic completeness is to introduce auxiliary wave operators such that "effective" perturbations are decaying functions. This requires a suitable smooth partition of unity. Moreover, it is convenient to choose auxiliary identifications as first-order differential operators rather than operators of multiplication. Unfortunately, although such identifications allow one to "kill" directions where the potentials $V^{\alpha}(x^{\alpha})$ do not tend to zero, their commutators with the operator H_0 have coefficients decaying at infinity only as $|x|^{-1}$.

Thus, we introduce differential operators

$$M_a = -\mathrm{i} \sum \left(m_a^{(j)} \partial_j + \partial_j m_a^{(j)} \right)$$

with coefficients $m_a^{(j)} = \partial m_a / \partial x_j$. The functions m_a satisfy properties (1), (2) formulated above and

5. $m_a(x) = 0$ in some conical neighborhoods of the subspaces X_b such that $X_a \not\subset X_b$. To put it differently, $m_a(x) = 0$ in some conical neighborhood of the subspace where $x_i = x_j$ for some i, j belonging to different clusters $\mathcal{C}_1, \ldots, \mathcal{C}_n$.

Let the operator H_a be defined by eqn [9]. Given the limiting-absorption principle and the radiation estimates, we first check the existence of auxiliary wave operators

$$W^{\pm}(H, H_a; M_a E_a(\Lambda))$$

and

$$W^{\pm}(H_a, H; M_a E(\Lambda)) \qquad [25]$$

Here we use that according to (5) coefficients of the differential operator $(V - V^a) M_a$ are, under assumption [11], short-range (in the configuration space X^{cm}). By property (2), the function $[V^a, M_a]$ is also short-range. Thus, the operator $V M_a - M_a V^a$ can be taken into account by the limiting-absorption principle. The commutator $[H_0, M_a]$ factorizes into a product of H_a- and H-smooth operators according to the radiation estimates.

Similar arguments show that, for $\sum_a m_a = m$ and $M = \sum_a M_a$ (the sums here are taken over all possible breakups of the N-particle system), the wave operator (observable)

$$W^{\pm}(H, H; \pm M E(\Lambda)) \qquad [26]$$

also exists. Moreover, it can be easily achieved that $m(x) \geq 1$. Then it follows from the Mourre estimate that operator [26] is positive definite on the subspace $E(\Lambda)\mathcal{H}$ and hence its range coincides with this subspace. It means that for all $f \in E(\Lambda)\mathcal{H}$

$$\lim_{t \to \pm\infty} \| \exp(-\mathrm{i}Ht) f - M \exp(-\mathrm{i}Ht) g^{\pm} \| = 0 \qquad [27]$$

if $f = W^{\pm}(H, H; M E(\Lambda)) g^{\pm}$.

The existence of wave operators [25] implies that for any $g^{\pm} = E(\Lambda) g^{\pm}$ and $g_a^{\pm} = W^{\pm}(H_a, H; M_a E(\Lambda)) g^{\pm}$

$$\lim_{t \to \pm\infty} \| M \exp(-\mathrm{i}Ht) g^{\pm} - \sum_a \exp(-\mathrm{i}H_a t) g_a^{\pm} \| = 0 \qquad [28]$$

Combining eqns [27] and [28], we see that $\exp(-\mathrm{i}Ht)f$ decomposes asymptotically into simpler evolutions $\exp(-\mathrm{i}H_a t) g_a^{\pm}$. This is one of the equivalent formulations of asymptotic completeness and leads to eqn [15].

Finally, we note that eqn [15] can be rewritten as

$$\exp(-\mathrm{i}Ht)f = \sum_a \exp(\mathrm{i}\Phi_a(x_a, t))(2\mathrm{i}t)^{-d_a/2} \times \hat{f}_a^{\pm}(x_a/(2t)) \psi^a(x^a) + o(1) \qquad [29]$$

where $t \to \pm\infty$, $d_a = \dim X_a$, $\hat{f}_a^{\pm}$ is the Fourier transform of $f_a^{\pm}$ and

$$\Phi_a(x_a, t) = x_a^2(4t)^{-1} - \lambda^a t \qquad [30]$$

Long-Range Interactions: New Channels

The multiparticle problem acquires a long-range character if pair potentials decay as Coulomb potentials or slower. Similarly to the two-particle problem, for long-range potentials the definition of wave operators should be naturally modified. As in the short-range case, only the asymptotic completeness is a really difficult mathematical problem. Assume that pair potentials satisfy condition

$$|(\partial^{\kappa} V^{\alpha})(x^{\alpha})| \leq C(1 + |x^{\alpha}|)^{-\rho-|\kappa|}, \quad \rho > \sqrt{3} - 1$$

for all $|\kappa| \leq \kappa_0$ and sufficiently large κ_0. Then only phase factors in eqn [29] should be modified. Actually, instead of eqn [30] we should set

$$\Phi_a(x_a, t) = x_a^2(4t)^{-1} - \lambda^a t - t\int_0^1 V_a(sx_a, 0)\,ds$$

where $V_a(x) = V(x) - V^a(x)$ and as usual $x = (x_a, x^a)$. As shown in Dereziński (1993), with this definition of wave operators, the asymptotic completeness holds.

On the contrary, if pair potentials decay slower than $|x|^{-1/2}$, then the traditional picture of scattering breaks down (see Yafaev (1996)). Actually, a three-particle system might have additional scattering channels intermediary between the channel where three particles are asymptotically free and the channels where a couple of particles form a bound state. In these additional channels, the bound state of a couple of particles depends on a position of the third particle, and it is destroyed asymptotically.

See also: Quantum Mechanical Scattering Theory; Schrödinger Operators.

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Nuclear Magnetic Resonance

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Introduction

The existence of nuclear spin and its associated magnetism was first suggested by Wolfgang Pauli in 1924, a conjecture based on the fine details of atomic spectra, the so-called hyperfine structure. The interaction of this nuclear magnetism with an external magnetic field was predicted to result in a finite number of discrete energy levels known as the Zeeman structure. However, the first direct excitation of transitions between nuclear Zeeman levels was by Isador Rabi in 1933, using radiofrequency (RF) waves in an atomic beam apparatus. In 1945, Felix Bloch and co-workers at Stanford, and Edward Purcell and co-workers at MIT, performed the first nuclear magnetic resonance (NMR) experiments in condensed matter, with the RF response of the hydrogen nucleus (proton) being directly detected.

The early prospects for this new technique were limited to precise measurements of magnetic fields and nuclear magnetic moments. However, three transformational discoveries intervened to set NMR on a course that would result in initially unimaginable contributions to physics, chemistry,

engineering, medicine, geology, food science, and biochemistry. In 1950, it was found that atomic nuclei at different sites of a molecular orbital had slightly different resonant frequencies, a phenomenon known as "chemical shift." In the a same year, Erwin Hahn discovered the spin echo, thus opening the possibility that multiple RF pulse trains could be used to remove unwanted nuclear spin interactions while being used to manipulate spin coherences with exquisite resolution. In addition, in 1951, using this spin echo, Herbert Gutowsky and Charles Slichter revealed a hitherto unobserved scalar spin–spin interaction between nuclei, mediated by the molecular orbital electrons.

The discovery of the chemical shift and the scalar coupling would immediately revolutionize chemistry. Further discoveries of nuclear quadrupole interactions and through-space dipolar interactions would add to the capacity of NMR to provide insight regarding structure and order in the solid and liquid crystalline state. But the spin echo would provide a platform for new advances in science in every one of the six decades following the discovery of NMR in 1945. These were successively diffusion and flow NMR, multidimensional NMR, magnetic resonance imaging, protein structure NMR, *ex situ* NMR, and quantum computing NMR.

Resonant Excitation and Detection

In quantum-mechanical language, the Zeeman Hamiltonian H for a nuclear spin experiencing a magnetic field $\mathbf{B}_0$ along the laboratory z-axis may be written as

$$H = -\gamma B_0 I_z \qquad [1]$$

γ being the (nuclear) gyromagnetic ratio while I_z is the operator for the z-component of angular momentum, with eigenvalues $m\hbar$, m lying in the range $-I, -I+1, \ldots, I$. I is the angular momentum quantum number, being either integer or half-integer. From the Schrödinger equation, it can be seen that the eigenkets of H precess about the z-axis at a rate γB_0, the frequency corresponding to the energy difference between the $2I+1$ Zeeman levels. For convenience, we shall take the eigenvalues of I_z to be simply m, dropping the factor $\hbar$, and leading to a Hamiltonian expressed in frequency rather than in energy units.

Resonant excitation between the Zeeman levels is achieved by the application of an RF (ω) magnetic field of amplitude $2B_1$ linearly polarized normal to $\mathbf{B}_0$ such that the total Hamiltonian becomes

$$H = -\gamma B_0 I_z - 2\gamma B_1 \cos \omega t I_x \qquad [2]$$

This excitation is easily applied by means of a transversely oriented antenna coil, the same coil generally being used to detect the nuclear spin response. In the frame of reference rotating about $\mathbf{B}_0$ at ω, the Hamiltonian transforms to

$$H = -\gamma\left(B_0 - \frac{\omega}{\gamma}\right)I_z - \gamma B_1 I_x - \gamma B_1 \exp(\mathrm{i}2\omega t I_z) I_x \exp(-\mathrm{i}2\omega t I_z) \qquad [3]$$

At resonance, $\omega = \omega_0 = \gamma B_0$. The last term in eqn [3] averages to zero and may be neglected (the Heisenberg condition) provided $\omega \gg \gamma B_1$, that is, $B_0 \gg B_1$. Given B_0 of the order of tesla and B_1 of the order of millitesla, this condition is easily satisfied. Hence, from the perspective of the rotating frame, the spins at resonance see only the static magnetic interaction $\gamma B_1 I_x$, so that application of this resonant RF field causes spins to nutate about the rotating frame x-axis at a rate γB_1. Thus, by application of RF pulses of different duration, and phases, one may produce arbitrary reorientation of the spins about various axes in the rotating frame.

With the spin system disturbed from equilibrium, the NMR "signal" is detected via the subsequent free precession, and usually via the same antenna coil used for resonant excitation, Semiclassically, the phenomenon may be pictured as follows. RF excitation nutates an initial z-magnetization into the transverse plane of the rotating frame. Such transverse magnetization corresponds the laboratory frame to a magnetization precessing at the Larmor frequency, thus inducing an oscillating emf in the receiver coil. In the next section, we see how to describe this phenomenon in the language of quantum mechanics.

Typically, NMR is performed using the nuclei of common atoms in organic molecules, (^{1}H, ^{2}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P) although for inorganic matter a wider class of nuclei are available. Of all these, the proton is most abundant and most sensitive, having the highest gyromagnetic ratio, γ, of all stable nuclei.

The Quantum Statistics of the Spin Ensemble

The nuclear Zeeman energy in typically available laboratory magnetic fields, $\gamma B_0 \hbar$, is many orders of magnitude smaller than the Boltzmann energy, $k_B T$, except at millikelvin temperatures. At room temperature in thermal equilibrium, the fractional difference in populations between the Zeeman levels

is normally very small, for example, for protons, about 10^{-5}. Of course, the total number of spins available may be very large, for example, on the order of 10^{20}.

The signal in magnetic resonance is detected as a collective effect of the large ensemble of nuclear spins. The natural language of quantum statistics is that of the density matrix, ρ; the time-dependent expectation value for any observable represented by an operator O is then, $\mathrm{tr}(O\rho(t))$, the diagonal sum of the product of O and ρ. The time evolution of the density matrix is given by the Liouville equation

$$\mathrm{i}\frac{\partial \rho}{\partial t} = [H, \rho] \qquad [4]$$

where [,] is a commutator. For a constant Hamiltonian, this equation gives

$$\rho(t) = \exp(\mathrm{i}Ht)\rho(0)\exp(-\mathrm{i}Ht) \qquad [5]$$

Physical solutions to the density matrix (Liouville space) are $(2I+1)^2$ (square) matrices formed in the $(2I+1)$-dimensional angular momentum eigenbasis. Generally, we may write the density matrix in a representation of irreducible tensor operators. One very convenient representation is the set formed by taking products of spin operators. For example, in the case of spin-1/2 where Liouville space is 2^2-dimensional, we may write

$$\rho(t) = \tfrac{1}{2}I + a_x I_x + a_y I_y + a_z I_z \qquad [6]$$

where I is the identity operator. The operators I_x and I_y provide the off-diagonal elements of ρ and define the degree of phase coherence in the ensemble, while the operator I_z defines the degree to which the diagonal elements differ, thus defining the polarization. a_x and a_y give the amount of "one-quantum coherence" in the ensemble while a_z gives the polarization. In thermal equilibrium $a_x = a_y = 0$, and the spin ensemble exists in a state of pure longitudinal polarization given, in the high-temperature approximation, $\gamma B_0 \hbar << k_B T$, by

$$\rho_{\mathrm{eqbm}}(0) \approx \frac{1}{(2I+1)} I + \frac{\gamma \hbar B_0}{(2I+1)k_B T} I_z \qquad [7]$$

This is the starting point for all NMR experiments (**Figure 1**).

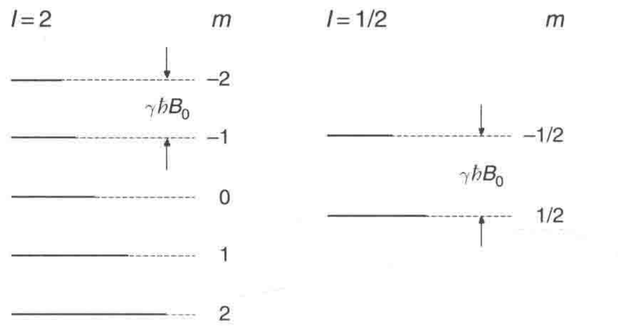


Figure 1 Schematic Zeeman levels for the case $I = 2$ *and* $I = 1/2$. The bold lines indicate the relative population in each state in thermal equilibrium.

Consider then the detection of precession via the Faraday induction. The size of the signal observed will be proportional to the size of the transverse magnetization $M = \mathrm{tr}[(I_x + \mathrm{i}I_y)\rho(t)]$ present in the rotating frame, this magnetization producing an induced emf with real and imaginary components because of the capacity of heterodyne receivers to detect quadrature phase. In the laboratory frame, the detected signal has a prefactor of γB_0 reflecting the Faraday induction, which, taken together with the dependence of the initial equilibrium magnetization on γB_0, gives an overall NMR sensitivity $(\gamma B_0)^2$, helping to explain in part why high magnetic fields are advantageous. Take the simple example for $I = 1/2$, where a single 90° resonant RF pulse is applied to the spin system, subsequent free precession occurring under the Zeeman Hamiltonian. The density matrix at detection is

$$\begin{aligned}
\rho(t) &= \exp(\mathrm{i}\omega_0 t I_z)\exp\left(\mathrm{i}\frac{\pi}{2}I_x\right)\rho_{\mathrm{eqbm}}(0) \\
&\quad \times \exp\left(-\mathrm{i}\frac{\pi}{2}I_x\right)\exp(-\mathrm{i}\omega_0 t I_z) \\
&= \exp(\mathrm{i}\omega_0 t I_z)\exp\left(\mathrm{i}\frac{\pi}{2}I_x\right)a_{\mathrm{eqbm}} I_z \\
&\quad \times \exp\left(-\mathrm{i}\frac{\pi}{2}I_x\right)\exp(-\mathrm{i}\omega_0 t I_z) \\
&= \exp(\mathrm{i}\omega_0 t I_z)a_{\mathrm{eqbm}} I_y \exp(-\mathrm{i}\omega_0 t I_z) \\
&= a_{\mathrm{eqbm}} I_y \cos(\omega_0 t) + a_{\mathrm{eqbm}} I_x \sin(\omega_0 t)
\end{aligned} \qquad [8]$$

Noting $\mathrm{tr}(I_x^2) = \mathrm{tr}(I_y^2) = \mathrm{tr}(I_z^2) = (1/3)(2I+1)I(I+1)$ and $\mathrm{tr}(I_\alpha I_\beta) = 0$, the signal may easily be calculated as $S(t) : a_{\mathrm{eqbm}} \exp(\mathrm{i}\omega_0 t)$, corresponding, upon Fourier transformation, to a unique frequency at ω_0. Note that a basis consisting of products of angular momentum operators are easy to handle since all evolution properties follow from the usual angular momentum commutation algebra.

The spin echo pulse scheme of **Figure 2** is one of the most important in NMR. It allows one to refocus dephasing effects caused by inhomogeneous broadening, for example, due to the heterogeneity of the magnetic field across the sample. Rewriting the density matrix equation in the rotating frame, replacing the Zeeman precession

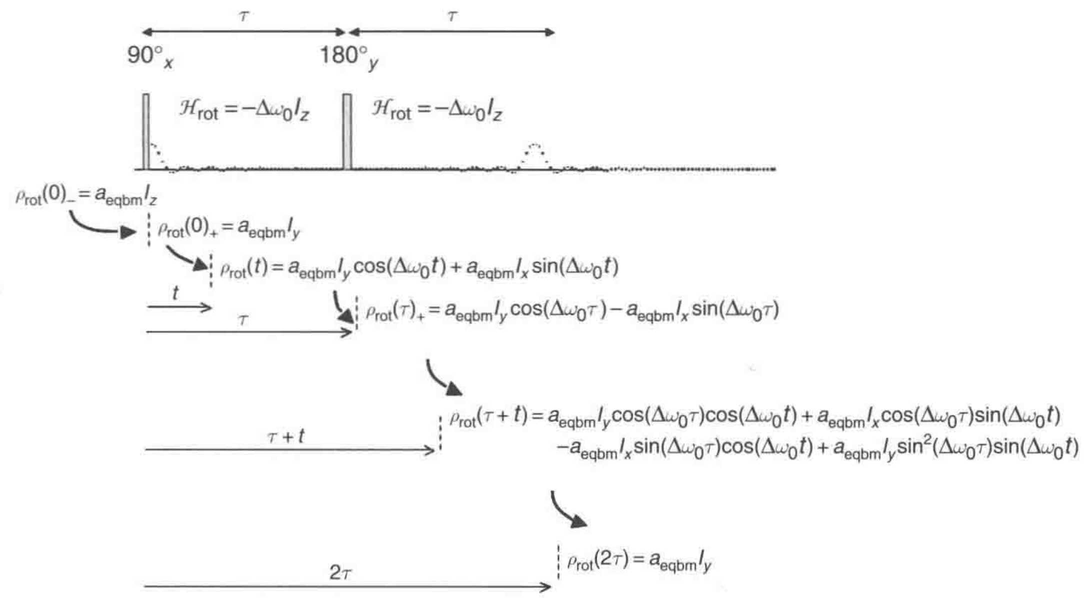


Figure 2 Spin echo pulse scheme showing the evolution of the density matrix.

by its residual offset, and accounting for both RF pulses,

$$\begin{aligned}\rho_{\text{rot}}(2\tau) &= \exp(\mathrm{i}\Delta\omega_0\tau I_z)\exp(\mathrm{i}\pi I_y)\exp(\mathrm{i}\Delta\omega_0\tau I_z) \\ &\quad\times \exp\left(\mathrm{i}\frac{\pi}{2}I_x\right)\rho_{\text{eqbm}}(0)\exp\left(-\mathrm{i}\frac{\pi}{2}I_x\right) \\ &\quad\times \exp(-\mathrm{i}\Delta\omega_0\tau I_z)\exp(-\mathrm{i}\pi I_y) \\ &\quad\times \exp(-\mathrm{i}\Delta\omega_0\tau I_z) \\ &= a_{\text{eqbm}}I_y \end{aligned} \qquad [9]$$

Details of the density matrix evolution are given in **Figure 2**. The inversion pulse has the effect of completely reversing all the phase shifts that occur during the first interval, resulting in an echo signal when the two time periods are equal. Note the use of nested operators representing the successive influences of RF pulses (assumed to be ideal rotations) and Hamiltonian evolutions. The overall influence of the RF pulses is to render the effective Hamiltonian zero in this case.

This echo sequence (and its equivalent multiple RF train, the Carr–Purcell–Meiboom–Gill sequence) allows one to remove the effect of magnetic field inhomogeneities so as to investigate the underlying homogeneous broadening and associated signal damping.

Spin Relaxation

The free precession of nuclear spins does not continue indefinitely. Ultimately the off-diagonal elements of the density matrix lose phase coherence while the diagonal elements gradually return to their thermal equilibrium state, two processes known, respectively, as T_2 (spin–spin) and T_1 (spin–lattice) relaxation. The rate of relaxation depends on interactions between the spins themselves and between the spins and their thermal environment. The process of T_1 relaxation requires fluctuations that induce transitions between the Zeeman levels. Clearly the relevant quantum-mechanical operators must possess a nonzero matrix element coupling the Zeeman levels, and the frequency of those fluctuations must match the energy gap spacing. Predominant in causing such relaxation in diamagnetic environments are the internuclear dipolar interactions, while in paramagnetic environments, dipolar interactions between nuclear and electronic spins are effective. One simple way of representing these processes is by the spectral density function, the Fourier power transform of their fluctuations, dipolar interactions causing spin–lattice relaxation due to fluctuations at ω_0 and $2\omega_0$. For a fluctuating interaction with correlation time, τ_c, that spectral density may approximate a Lorentzian of the form

$$J(\omega) = \frac{\tau_c}{1 + \omega^2\tau_c^2} \qquad [10]$$

Thus, as the rate of molecular motions varies, due to the influence of temperature on τ_c, the T_1 relaxation rate will be a maximum when $\omega_0\tau_c = 1$. Both solids ($\omega_0\tau_c \gg 1$) and liquids ($\omega_0\tau_c \ll 1$) have long T_1 relaxation times while soft solids or complex liquids may have faster relaxation. T_1 relaxation manifests as an exponential return to equilibrium values of longitudinal magnetization. Typical vales range from hundreds of milliseconds to hours, and the need to re-establish equilibrium between repetitions of the experiment can severely limit signal averaging

and hence available signal-to-noise ratios. Note that T_1 relaxation occurs by stimulated emission. Spontaneous emission is effectively absent from nuclear spin systems owing to the long-radiation wavelength.

The case of T_2 (spin–spin) relaxation is inherently more complex. First, the definition of "loss of phase coherence" depends on the particular RF pulse sequence employed. Second, the simple perturbation theory description applied to T_1 relaxation only works in the fast motion limit, where the T_2 relaxation rate may be shown to depend on spectral density terms not only at ω_0 and $2\omega_0$ but also $\omega = 0$. In consequence, $T_2 \ll T_1$. T_2 relaxation is sensitive to static components. These static components may dominate in soft solids and solids. Indeed, any term in the Hamiltonian which spreads spin phases, and which cannot be recovered by means of a judicious RF pulse train, will contribute to T_2 relaxation. Suppose the effective frequency distribution causing dephasing is described by an ensemble second moment $<\Delta\omega^2>$, and exhibits fluctuations about a mean of zero with correlation time, τ_c. Then we may identify two limiting cases: in the slow motion limit $<\Delta\omega^2>^{1/2}\ \tau_c \gg 1$, the decay of the detected magnetization is Gaussian, and given by a factor $\exp(-1/2 <\Delta\omega^2> t^2)$. In solids, the proton T_2 relaxation may take place in a few tens of microseconds. In the fast motion limit $<\Delta\omega^2>^{1/2}\ \tau_c \ll 1$, the decay of the detected magnetization is exponential, and given by a factor $\exp(-<\Delta\omega^2>\tau_c t)$. Liquid state T_2 values approach T_1 under extreme narrowing conditions.

The Details of the Nuclear Spin Hamiltonian

Atomic nuclei interact with their environment, with surrounding electrons, and with other nuclear spins. It is precisely this feature that provides such a sensitive probe of material structure and dynamics. For a material immersed in a steady magnetic field $\boldsymbol{B}_0$ along the laboratory z-axis, the Hamiltonian for the ith nuclear spin can be written

$$H = -\gamma B_0 I_{iz} - \boldsymbol{I}_i.\underline{\underline{S}}.\boldsymbol{B}_0 + \sum_j J\boldsymbol{I}_i.\boldsymbol{I}_j + \sum_j \boldsymbol{I}_i.\underline{\underline{D}}.\boldsymbol{I}_j + \boldsymbol{I}_i.\underline{\underline{Q}}.\boldsymbol{I}_i \qquad [11]$$

It is the variety of the terms in the nuclear spin Hamiltonian that imparts power to NMR. The first is the nuclear Zeeman interaction with the applied magnetic field. In modern laboratory superconducting magnets, this interaction can be as large as 1000 MHz, although in earth field applications it can be as small as 2.5 kHz. Given that the sensitivity and resolution of NMR generally improve with increasing magnetic field, the range of 100–1000 MHz is typically the operating regime of choice. All other terms in the nuclear spin Hamiltonian are smaller and thus act as first-order perturbations only, projecting their quantum operators into the zeroth-order Zeeman eigenbasis, the quantum frame of the operator I_z. Because several of the terms in H depend on the orientation of the local nuclear environment (e.g., the molecular orbital) with respect to the magnetic field, these terms will fluctuate in the presence of reorientational motions. By the Heisenberg uncertainty principle, fluctuations faster in frequency than the size of the Hamiltonian contribution, expressed in frequency units, will result in an averaging to the mean, a phenomenon known as "motional averaging."

The term $-\boldsymbol{I}_i.\underline{\underline{S}}.\boldsymbol{B}_0$ is the chemical shift that occurs for nuclei in molecular atoms, or the knight shift for nuclei in metals. It is typically a few ppm to several 100 ppm (i.e., 100's Hz to 10 kHz), depending on the nucleus. $\underline{\underline{S}} = \gamma\underline{\underline{\sigma}}$ is a tensor whose principal axes (1, 2, 3) are associated with the local symmetry axis of the molecular orbital (bond) in the vicinity of the nucleus. For a liquid state molecule tumbling rapidly and isotropically, only the averaged trace of $\underline{\underline{\sigma}}, \sigma_i = (1/3)(\sigma_{11} + \sigma_{22} + \sigma_{33})$ survives under motional averaging, giving a fixed frequency shift $-\sigma_i \gamma B_0 I_{iz}$. However, in a solid-state environment, the remaining terms also contribute to the anisotropic chemical shift

$$H_{CS} = -\sigma_i \gamma B_0 I_{iz} - \tfrac{1}{2}(3\cos^2\beta - 1) \times (\sigma_{33} - \sigma_i)\gamma B_0 I_{iz} \qquad [12]$$

where β is the polar angle between the magnetic field and the principal axis (the axis "3").

The scalar coupling term, $\sum_j J\boldsymbol{I}_i.\boldsymbol{I}_j$ causes each (ith spin) energy level to be sensitive to the quantum states of the neighboring j-spins, the coupling constant J being typically tens to hundreds of hertz for nearby spins, but reducing rapidly with greater distance in the molecular orbital. Note that the operator $\sum_j J\boldsymbol{I}_i.\boldsymbol{I}_j$ is nondiagonal in the zeroth-order representation, but provided that the chemical shift between the I and j spins is larger than the coupling frequency (known in chemistry as an AX spin system), the operator reduces to $\sum_j J I_{iz} I_{jz}$ the effect being to split the i-spin resonance in to a multiplet, depending on the state of the nearby j-spin. For m identical nearby j-spins, the multiplet bears a simple

binomial relationship to m, allowing one to "read" this number directly. The combination of chemical shift and scalar coupling information is of profound importance in identifying molecular structure in chemistry.

The terms $\sum_j \boldsymbol{I}_i.\underline{\underline{D}}.\boldsymbol{I}_j$ and $\boldsymbol{I}_i.\underline{\underline{Q}}.\boldsymbol{I}_i$ are, respectively, the through-space dipolar interaction, H_D, and the nuclear quadrupole interaction, H_Q, the latter being nonzero only for nuclear spin quantum numbers $I \geq 1/2$, for example, ^{2}H. These interactions, projected into the zeroth-order Zeeman frame, for the dipole–dipole interaction, are

$$H_\mathrm{D} = \frac{\mu_0 \hbar}{4\pi} \sum_{j>i} \frac{\gamma_i \gamma_j}{r_{ij}^3} \frac{1}{2} (1 - 3\cos^2\theta_{ij}) \times (3I_{iz}I_{jz} - \boldsymbol{I}_i.\boldsymbol{I}_j) \qquad [13]$$

where r_{ij} is the internuclear distance and θ_{ij} is the angle made by the internuclear vector with the magnetic field direction; while, for the quadrupole interaction

$$H_\mathrm{Q} = \frac{3eV_{ZZ}Q}{4I(2I-1)\hbar} \frac{1}{2} (1 - 3\cos\theta_{ZZ}) \times (3I_z^2 - I(I+1)) \qquad [14]$$

where Q is the nuclear quadrupole moment, V_{ZZ} is the electric field gradient (assuming axial symmetry) and θ_{ZZ} is the angle made by the principal axis of that gradient with the magnetic field direction. For protons in organic matter, the internuclear dipole interaction strength is on the order of 100 kHz, a similar strength being found for the quadrupole interaction of deuterons. However, in the liquid state, these orientation-dependent interactions fluctuate so rapidly that they are typically motionally averaged to zero. Nonetheless, their fluctuations do contribute to the relaxation process.

Liquid-state NMR can result in exceptionally high-resolution (sub-Hz) spectra, if care is taken to adjust the magnetic field harmonics (shims) to produce a highly uniform Zeeman field across the sample. The last contribution of residual inhomogeneities to line broadening can often be removed by gently spinning the sample about its axis at a rate of a few tens of hertz.

The Evolution Domain, Multiple RF Pulses, and Multidimensional NMR

Having seen the complexity of the spin Hamiltonian, one may envisage experiments where the spin coherences evolve in a much more complicated manner. To this end, consider the case of a molecular liquid two-spin (AX) system coupled via the scalar spin–spin interaction. In first-order perturbation theory, we may represent the simple two-spin Hamiltonian (in the rotating frame of the averaged Larmor frequency) as

$$\begin{aligned} H_\mathrm{rot} &= -\sigma_1 \gamma B_0 I_{1z} - \sigma_2 \gamma B_0 I_{2z} + J I_{1z} I_{2z} \\ &= -\omega_1 I_{1z} - \omega_2 I_{2z} + J I_{1z} I_{2z} \end{aligned} \qquad [15]$$

We now write down the density matrix in the rotating frame following a single 90°_x RF pulse (I_x),

$$\begin{aligned} \rho(t) &= \exp(\mathrm{i}\omega_1 t I_{1z} + \mathrm{i}\omega_2 t I_{2z} + \mathrm{i}J I_{1z} I_{2z} t) \\ &\quad \times \exp\left(\mathrm{i}\frac{\pi}{2} I_x\right) a_\mathrm{eqbm}(I_{1z} + I_{2z}) \exp\left(-\mathrm{i}\frac{\pi}{2} I_x\right) \\ &\quad \times \exp(-\mathrm{i}\omega_1 t I_{1z} - \mathrm{i}\omega_2 t I_{2z} - \mathrm{i}J I_{1z} I_{2z} t) \\ &= \exp(\mathrm{i}\omega_1 t I_{1z} + \mathrm{i}\omega_2 t I_{2z} + \mathrm{i}J I_{1z} I_{2z} t) a_\mathrm{eqbm}(I_{1y} + I_{2y}) \\ &\quad \times \exp(-\mathrm{i}\omega_1 t I_{1z} - \mathrm{i}\omega_2 t I_{2z} - \mathrm{i}J I_{1z} I_{2z} t) \\ &= \exp(\mathrm{i}\omega_1 t I_{1z} + \mathrm{i}\omega_2 t I_{2z}) a_\mathrm{eqbm} \\ &\quad \times \left((I_{1y} + I_{2y})\cos\left(\tfrac{1}{2}Jt\right) + 2(I_{1z}I_{2x} + I_{1x}I_{2z}) \right. \\ &\quad \left. \times \sin\left(\tfrac{1}{2}Jt\right)\right) \exp(-\mathrm{i}\omega_1 t I_{1z} - \mathrm{i}\omega_2 t I_{2z}) \\ &= a_\mathrm{eqbm} \begin{pmatrix} (I_{1y}\cos\omega_1 t + I_{2y}\cos\omega_2 t \\ \quad + I_{1x}\sin\omega_1 t + I_{2x}\sin\omega_2 t)\cos\left(\tfrac{1}{2}Jt\right) \\ \quad + 2(I_{1z}I_{2x}\cos\omega_2 t - I_{1z}I_{2y}\sin\omega_2 t \\ \quad + I_{1x}I_{2z}\cos\omega_1 t - I_{1y}I_{2z}\sin\omega_1 t) \\ \quad \times \sin\left(\tfrac{1}{2}Jt\right) \end{pmatrix} \end{aligned} \qquad [16]$$

Detection in the rotating frame with $I_x + \mathrm{i}I_y$ gives a signal

$$S(t) \sim a_\mathrm{eqbm}(\exp(\mathrm{i}\omega_1 t) + \exp(\mathrm{i}\omega_2 t))\cos\left(\tfrac{1}{2}Jt\right) \qquad [17]$$

Fourier transformation with respect to t yields a spectrum corresponding to two spectral lines at ω_1 and ω_2, each split into a doublet of two sidebands separated by J.

Notice that it is easier to follow the evolution of the density matrix by simply writing down a time sequence of behaviors under the influence of the successive Hamiltonians. Where simultaneous terms in the Hamiltonians commute, the order of their operation may be set at will. Thus, the above example becomes

$$\begin{aligned} I_{1z} + I_{2z} &\xrightarrow{\frac{\pi}{2}I_x} I_{1y} + I_{2y} \xrightarrow{JI_{1z}I_{2z}t} (I_{1y} + I_{2y})\cos\left(\tfrac{1}{2}Jt\right) \\ &\quad + 2(I_{1z}I_{2x} + I_{1x}I_{2z})\sin\left(\tfrac{1}{2}Jt\right) \\ &\xrightarrow{\omega_1 t I_{1z} + \omega_2 t I_{2z}} (I_{1y}\cos\omega_1 t + I_{2y}\cos\omega_2 t \\ &\quad + \mathrm{i}I_{1x}\sin\omega_1 t + \mathrm{i}I_{2x}\sin\omega_2 t)\cos\left(\tfrac{1}{2}Jt\right) \\ &\quad + 2(I_{1z}I_{2x}\cos\omega_2 t - \mathrm{i}I_{1z}I_{2y}\sin\omega_2 t \\ &\quad + I_{1x}I_{2z}\cos\omega_1 t - \mathrm{i}I_{1y}I_{2z}\sin\omega_1 t)\sin\left(\tfrac{1}{2}Jt\right) \end{aligned} \qquad [18]$$

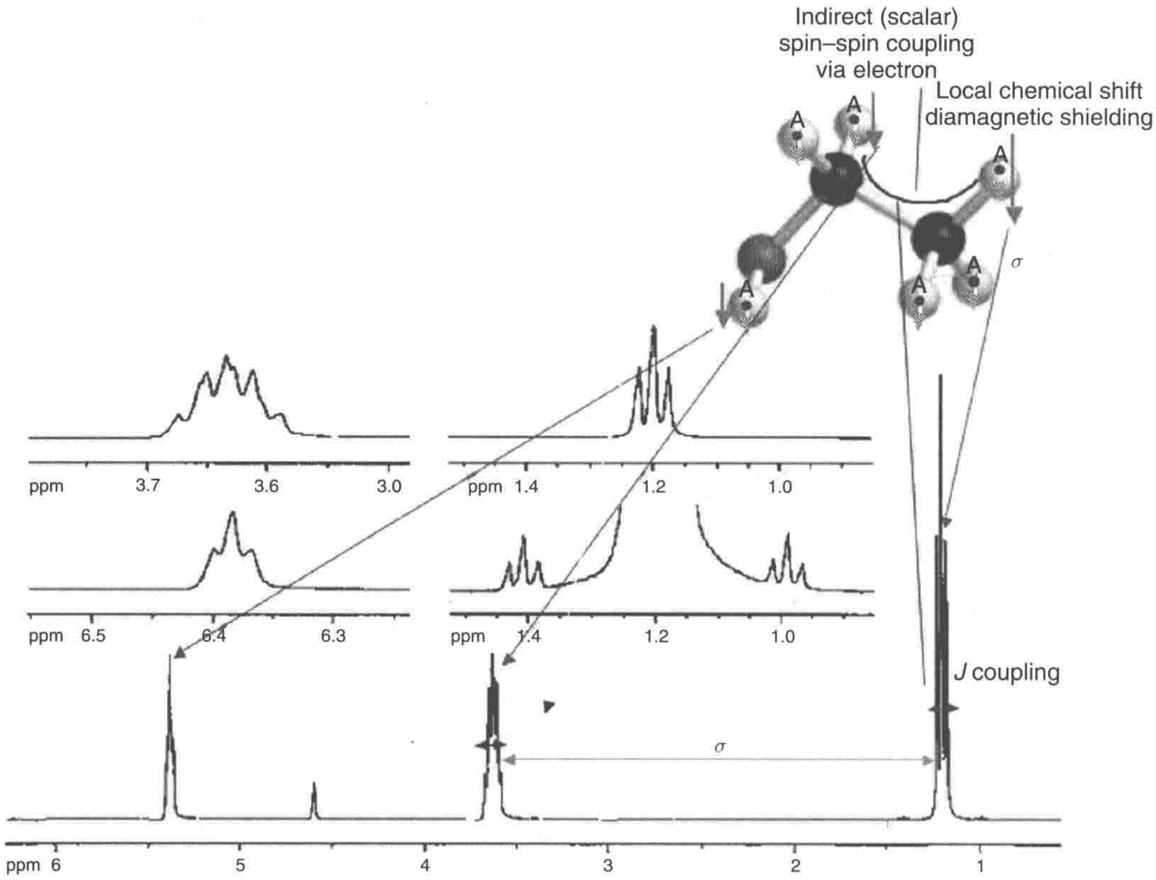


Figure 3 The proton NMR spectrum of ethanol showing three major peaks, separated by chemical shift, each split into multiplets arising from nearby protons via the scalar coupling.

Now consider a two RF pulse scheme as shown in **Figure 4**, each RF pulse being $90°_x$. The evolution is

$$I_{1z} + I_{2z} \xrightarrow{\frac{\pi}{2}I_x} I_{1y} + I_{2y} \xrightarrow{\omega_1 t_1 I_{1z} + \omega_2 t_1 I_{2z} - J I_{1z} I_{2z} t_1} \big(I_{1y}\cos\omega_1 t_1 + I_{2y}\cos\omega_2 t_1 + I_{1x}\sin\omega_1 t_1 + I_{2x}\sin\omega_2 t_1\big)\cos\left(\tfrac{1}{2}Jt_1\right) + 2\big(I_{1z}I_{2x}\cos\omega_2 t_1 - I_{1z}I_{2y}\sin\omega_2 t_1 + I_{1x}I_{2z}\cos\omega_1 t_1 - I_{1y}I_{2z}\sin\omega_1 t_1\big)\sin\left(\tfrac{1}{2}Jt_1\right)$$

$$\xrightarrow{\frac{\pi}{2}I_x} (-I_{1z}\cos\omega_1 t_1 - I_{2z}\cos\omega_2 t_1 + I_{1x}\sin\omega_1 t_1 + I_{2x}\sin\omega_2 t_1)\cos\left(\tfrac{1}{2}Jt_1\right) + 2\big(I_{1y}I_{2x}\cos\omega_2 t_1 + I_{1y}I_{2z}\sin\omega_2 t_1 + I_{1x}I_{2y}\cos\omega_1 t_1 + I_{1z}I_{2y}\sin\omega_1 t_1\big)\sin\left(\tfrac{1}{2}Jt_1\right)$$

$$\xrightarrow[\text{Keeping only observable magnetization}]{\omega_1 t_2 I_{1z} + \omega_2 t_2 I_{2z} + J I_{1z} I_{2z} t_2} (I_{1x}\sin\omega_1 t_1\cos\omega_1 t_2 + I_{2x}\sin\omega_2 t_1\cos\omega_2 t_2) \times \cos\left(\tfrac{1}{2}Jt_1\right)\cos\left(\tfrac{1}{2}Jt_2\right) + (I_{1x}\sin\omega_2 t_1\sin\omega_1 t_2 + I_{2x}\sin\omega_1 t_1\sin\omega_2 t_2) \times \sin\left(\tfrac{1}{2}Jt_1\right)\sin\left(\tfrac{1}{2}Jt_2\right) \quad [19]$$

If the idealized experiment is performed with two independent time dimensions t_1 and t_2, then detection in the rotating frame over the t_2 period with $I_x + iI_y$ gives a signal (restricting our attention to the quadrant of positive frequencies)

$$S(t_1, t_2) \sim a_{\mathrm{eqbm}}(\exp(i\omega_1 t_1)\exp(i\omega_1 t_2) + \exp(i\omega_2 t_1) \times \exp(i\omega_2 t_2))\cos\left(\tfrac{1}{2}Jt_1\right)\cos\left(\tfrac{1}{2}Jt_2\right) + a_{\mathrm{eqbm}}(\exp(i\omega_2 t_1)\exp(i\omega_1 t_2) + \exp(i\omega_1 t_1)\exp(i\omega_2 t_2)) \times \sin\left(\tfrac{1}{2}Jt_1\right)\sin\left(\tfrac{1}{2}Jt_2\right) \quad [20]$$

When Fourier transformed in two dimensions with respect to t_1 and t_2, the pattern shown in **Figure 5** results. Remarkably, while the diagonal spectrum is the same pair of doublets seen in the figure, this two-dimensional spectrum contains off-diagonal antiphase peaks for scalar-coupled sites where magnetization transfer has occurred.

The idea of performing NMR in two or more dimensions was first proposed by Jean Jeener in 1971. The example outlined above, correlation spectroscopy (COSY), is just one of an array of coherence transfer experiments using multiple RF pulse trains and time domain evolution of the spin ensemble. Notice that in the COSY experiment, t_1 is an evolution dimension during which no detection of NMR signal occurs, while t_2 is the detection domain.

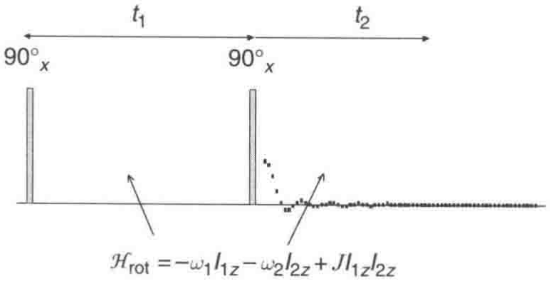


Figure 4 RF pulse scheme used for COSY experiment.

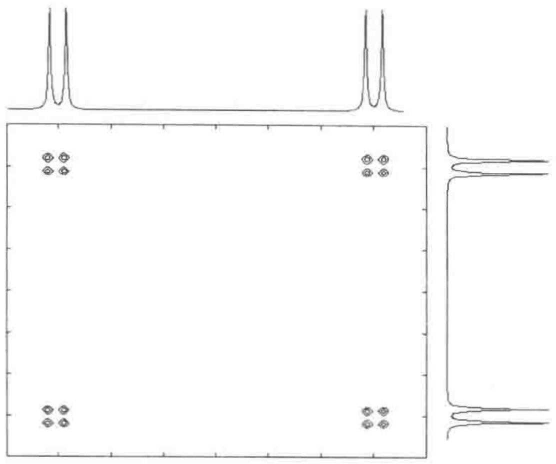


Figure 5 Schematic COSY (modulus) spectrum for an AX spin system. Not that the (antiphase) off-diagonal peaks indicate J-couplings between chemical-shift-separated spins.

The effect of the evolution is indelibly imprinted in the spin system density matrix allowing later recall of vital information concerning the interactions present in the spin Hamiltonian. The COSY experiment allows one to determine which spins are coupled via their molecular orbital electrons. Other multidimensional methods that rely on dipole–dipole relaxation effects, such as NOESY, determine which spin sites have "through-space" proximity.

The use of two- and higher-dimensional methods has allowed the NMR spectra of biological macromolecules to be unraveled, with COSY methods used for spectral assignment of amino acid units, and NOESY methods used to determine any close proximities of amino acids otherwise well separated in the sequence. Such distance information has allowed the reconstruction of protein conformations by NMR.

The second RF pulse of **Figure 4** also generates a state of the density matrix, $I_{1y}I_{2x}$ known as a double quantum coherence, and, in the simple COSY experiment, lost to observable magnetization. Other RF pulse schemes can take advantage of this state, converting it via suitable "coherence pathways" into an observable. For a detailed summary of these various NMR phenomena, readers are referred to the book by Ernst *et al.* (1987).

Solid-State NMR

As with J couplings, dipolar interactions and quadrupole interactions ($I > 1/2$) are bilinear in the spin operators and can be used to generate various higher-order coherence pathways in NMR experiments. Unlike the simple spin–spin coupling, they have an angular dependence. In solids, these interactions may broaden the NMR resonance line by tens to hundreds of kilohertz. In the case where a probe nucleus is located at a known site in the material (often achieved by deuteron labeling), these Hamiltonian terms may contribute important information about structure, and especially orientational anisotropy. For example, the quadrupole interaction for the spin-1 deuteron (see eqns [11] and [14]) depends as $P_2(\cos\theta_{ZZ}) = (1/2)(3\cos\theta_{ZZ} - 1)$ on the angle between the external magnetic field and the electric field gradient (generally associated with the local molecular orbital or bond direction, and taken here to be axially symmetric). Note that the first-order contribution of the quadrupole interaction leads to an unequal separation of the $m = 1, 0, -1$ Zeeman energy levels, resulting in a doublet NMR spectrum, for any particular orientation, θ_{ZZ}. Such a unique orientation might be found in a single crystal, or in a nematic liquid crystalline state. For a polycrystalline material, however, the NMR spectrum has a contribution from all orientations, leading to a characteristic powder pattern. The details of ^2H spectral distributions may be used to characterize the degree of orientational order in solids and soft, anisotropic matter.

For ^1H, ^{13}C, and other spin-1/2 nuclei, dipolar interactions (with a wide distribution of spin spacings and internuclear vector orientation) may severely broaden the NMR spectrum in the solid state (see eqns [11] and [13]). Such interactions, along with quadrupole interactions for nuclei with $I > 1/2$, may be significantly reduced by modulating the effective dipolar Hamiltonian at a rate faster than its strength in frequency units. Two methods are available, one (magic angle spinning or MAS) relying on the angular terms in eqns [13] and [14], and the other (multiple pulse line narrowing) on the spin terms. The MAS technique relies on spinning the sample rapidly about at angle oriented at 54.4° to the magnetic field, such that the average value of $P_2(\cos\theta_{ij})$ becomes its projection along this spinning axis, while the projection of the spinning axis residual is $P_2(\cos 54.4°) \approx 0$. Multiple pulse methods rely on a successive reorientation of the spin system such that the effective dipolar Hamiltonian that results from the application of the nested evolution operators is rendered close to zero.

In practice, MAS techniques work best with ^{13}C NMR where the moderate ^{1}H–^{13}C dipolar interactions may be removed with achievable spinning speeds (a few tens of kilohertz). Furthermore, the larger proton magnetization ($\gamma_{^1H}/\gamma_{^{13}C} \approx 4$) can be transferred to the ^{13}C nuclei via Hartman–Hahn cross-polarization thus significantly enhancing sensitivity. Such methodology is referred to as CPMAS NMR.

The real art of solid-state NMR is in removing the unwanted dipolar or quadrupolar interactions, but leaving specific interactions of interest. This may be achieved by including in the MAS experiment, specific combinations of pulses which recouple selected spins. Some of the most sophisticated experiments in modern NMR are to be found in this domain of application.

Conclusion

NMR provides exceptional structural information concerning molecules, biomolecules as well as molecular assemblies, liquid crystals, soft solids, and solids. In addition, the method provides unique information concerning molecular dynamics, through both relaxation methods and the direct measurement of diffusion or flow. One spectacular application of NMR concerns its use in imaging, achieved by giving the Larmor frequency a spatial tag through the use of deliberately inhomogeneous magnetic fields. This topic is covered in the article on Magnetic Resonance Imaging.

See also: Magnetic Resonance Imaging.

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Number Theory in Physics

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Several fields of mathematics have closely been associated to physics: this has always been the case for the theory of differential equations. In the early twentieth century, with the advent of general relativity and quantum mechanics, topics such as differential and Riemannian geometry, operator algebras, and functional analysis, or group theory also developed a close relation to physics. In the 1990s, mostly through the influence of string theory, algebraic geometry also began to play a major role in this interaction. Recent years have seen an increasing number of results suggesting that number theory also is beginning to play an essential part on the scene of contemporary theoretical and mathematical physics. Conversely, ideas from physics, mostly from quantum field theory and string theory, have started to influence work in number theory.

In describing significant occurrences of number theory in physics, we will, on the one hand, restrict our attention to quantum physics, while, on the other, we will assume a somewhat extensive definition of number theory that will allow us to include arithmetic algebraic geometry. The territory is vast and an extensive treatment would go beyond the size limits imposed by the encyclopedia. The choice of topics represented here inevitably reflects the limited knowledge, particular interests, and bias of the author. Very useful references, collecting a lot of material on number theory and physics, are the proceedings of the Les Houches conference in 2003 (Beilinson and Manin 1986), as well as the two volumes of a previous Les Houches conference on number theory and physics, which took place in 1989, published by Springer in 1990 and 1992. A number theory and physics database is presently maintained online by M R Watkins.

In the following, we have organized the material by topics in number theory that have so far made an appearance in physics, and for each we briefly describe the relevant context and results. This singles out many themes. We first discuss a class of functions that occur in physics and their special values that are of great number-theoretic importance. This includes the dilogarithm, the polylogarithms and multiple polylogarithms, and the multiple zeta values. We also discuss the most important symmetry groups of number theory, the Galois groups, and occurrences in physics of some forms of Galois theory. We then discuss how techniques from the arithmetic geometry of algebraic varieties, especially Arakelov geometry, play a role in string theory. Finally, we discuss briefly the theory of motives and outline its possible relation to quantum physics. From the physics point of view, it seems that the most promising directions in which number-theoretic tools have come to play a crucial role are to be found mostly in the realm of rational conformal field theories and of noncommutative geometry, as well as in certain aspects of string theory.

Among the topics that are very relevant to this theme, but that will not be touched upon in this article, there are important subjects such as the theory of "arithmetic quantum chaos," the use of methods of random matrix theory applied to the study of zeros of zeta functions, or mirror symmetry and its connection to modular forms. The interested reader can find such topics treated in other articles of this encyclopedia and in the references mentioned above (*see* Quantum Ergodicity and Mixing of Eigenfunctions; Random Matrix Theory in Physics; Mirror Symmetry: a Geometric Survey).

Dilogarithm, Multiple Polylogarithms, Multiple Zeta Values

The dilogarithm is defined as

$$Li_2(z) = \int_z^0 \frac{\log(1-t)}{t}\,dt = \sum_{n=1}^{\infty} \frac{z^n}{n^2}$$

It satisfies the functional equation $Li_2(z) + Li_2(1-z) = Li_2(1) - \log(z)\log(1-z)$, where $Li_2(1) = \zeta(2)$, for $\zeta(s)$ the Riemann zeta function. A variant is given by the Rogers dilogarithm $L(x) = Li_2(x) + (1/2)\log(x)\log(1-x)$. For more details, see Zagier's paper (Julia *et al.* 2005, vol. II).

The polylogarithms are similarly defined by the series $Li_k(z) = \sum_{n\geq 1} z^n/n^k$. In quantum electrodynamics, there are corrections to the value of the gyromagnetic ratio, in powers of the fine structure constant. The correction terms that are known exactly involve special values of the zeta function such as $\zeta(3), \zeta(5)$ and values of polylogarithms such as $Li_4(1/2)$. The series defining the polylogarithm function $Li_s(z) = \sum_{n\geq 1} z^n/n^s$ converges absolutely for all $s \in \mathbb{C}$ and $|z| < 1$ and has analytic continuation to $z \in \mathbb{C}\setminus[1,\infty)$. The Fermi–Dirac and Bose–Einstein distributions are expressed in terms of the polylogarithm function as

$$\int_0^\infty \frac{x^s}{e^{x-\mu} \pm 1}\,dx = -\Gamma(s+1)Li_{1+s}(\pm e^{\mu})$$

The multiple polylogarithms are functions defined by the expressions

$$Li_{s_1,\ldots,s_r}(z_1, z_2, \ldots, z_r) = \sum_{n_1>n_2>\cdots>n_r>0} \frac{z_1^{n_1} z_2^{n_2}\cdots z_r^{n_r}}{n_1^{s_1} n_2^{s_2}\cdots n_r^{s_r}} \qquad [1]$$

By analytic continuation, the functions $Li_{s_1,\ldots,s_r}(z_1, z_2, \ldots, z_r)$ are defined for all complex s_i and for z_i in the complement of the cut $[1,\infty)$ in the complex plane. Multiple zeta values of weight k and depth r are given by the expressions

$$\zeta(k_1, \ldots, k_r) = \sum_{n_1>n_2>\cdots>n_r>0} \frac{1}{n_1^{k_1}\cdots n_r^{k_r}} \qquad [2]$$

with $k_i \in \mathbb{N}$ and $k_1 \geq 2$. These satisfy many combinatorial identities and nontrivial relations over $\mathbb{Q}$. For an informative overview on the subject, see Cartier (2002). Notice that, for the sums in [1] and [2], a different summation convention can also be found in the literature.

Conformal Field Theories and the Dilogarithm

There is a relation between the torsion elements in the algebraic K-theory group $K_3(\mathbb{C})$ and rational conformally invariant quantum field theories in two dimensions (see Nahm (2005)). There is, in fact, a map, given by the dilogarithm, from torsion elements in the Bloch group (closely related to the algebraic K-theory) to the central charges and scaling dimensions of the conformal field theories.

This correspondence arises by considering sums of the form

$$\sum_{m\in\mathbb{N}^r} \frac{q^{Q(m)}}{(q)_m} \qquad [3]$$

where $(q)_m = (q)_{m_1}\cdots(q)_{m_r}$, $(q)_{m_i} = (1-q)(1-q^2)\cdots(1-q^{m_i})$ and $Q(m) = m^tAm/2 + bm + h$ has rational coefficients. Such sums are naturally obtained from considerations involving the partition function of a bosonic rational conformal field theory (CFT). In

particular, [3] can define a modular function only if all the solutions of the equation

$$\sum_j A_{ij} \log(x_j) = \log(1 - x_i) \qquad [4]$$

determine elements of finite order in an extension $\hat{B}(\mathbb{C})$ of the Bloch group, which accounts for the fact that the logarithm is multivalued. The Rogers dilogarithm gives a natural group homomorphism $(2\pi i)^2 L : \hat{B}(\mathbb{C}) \to \mathbb{C}/\mathbb{Z}$, which takes values in $\mathbb{Q}/\mathbb{Z}$ on the torsion elements. These values give the conformal dimensions of the fields in the theory.

Feynman Graphs

Multiple zeta values appear in perturbative quantum field theory. D Kreimer (2000) developed a connection between knot theory and a class of transcendental numbers, such as multiple zeta values, obtained by quantum field-theoretic calculations as counterterms generated by corresponding Feynman graphs. Broadhurst and Kreimer (1997) identified Feynman diagrams with up to nine loops whose corresponding counterterms give multiple zeta values up to weight 15. Recently, Kreimer showed some deep analogies between residues of quantum fields and variations of mixed Hodge–Tate structures associated to polylogarithms.

Testing predictions about the standard model of elementary particles, in the hope of detecting new physics, requires developing effective computational methods handling the huge number of terms involved in any such calculation, that is, efficient algorithms for the expansion of higher transcendental functions to a very high order. The interesting fact is that abstract number-theoretic objects, such as multiple zeta values and multiple polylogarithms, appear naturally in this context (cf., e.g., Moch *et al.* (2002)). The explicit recursive algorithms are based on Hopf algebras and produce expansions of nested finite or infinite sums involving ratios of gamma functions and Z-sums (Euler–Zagier sums), which naturally generalize multiple polylogarithms and multiple zeta values. Such sums typically arise in the calculation of multiscale multiloop integrals. The algorithms are designed to recursively reduce the Z-sums involved to simpler ones with lower weight or depth.

Galois Theory

Given a number field $\mathbb{K}$, which is an algebraic extension of $\mathbb{Q}$ of some degree $[\mathbb{K}:\mathbb{Q}] = n$, there is an associated fundamental symmetry group, given by the absolute Galois group $\mathrm{Gal}(\bar{\mathbb{K}}/\mathbb{K})$, where $\bar{\mathbb{K}}$ is an algebraic closure of $\mathbb{K}$. Even in the case of $\mathbb{Q}$, the absolute Galois group $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ is a very complicated object, far from being fully understood.

One can consider an easier symmetry group, which is the abelianization of the absolute Galois group. This corresponds to considering the field $\mathbb{K}^{ab}$, the "maximal abelian extension" of $\mathbb{K}$, which has the property that

$$\mathrm{Gal}(\mathbb{K}^{ab}/\mathbb{K}) = \mathrm{Gal}(\bar{\mathbb{K}}/\mathbb{K})^{ab}$$

The Kronecker–Weber theorem shows that for $\mathbb{K} = \mathbb{Q}$ the maximal abelian extension can be identified with the cyclotomic field (generated by all roots of unity), $\mathbb{Q}^{ab} = \mathbb{Q}^{\mathrm{cycl}}$, and the Galois group is identified with $\mathrm{Gal}(\mathbb{Q}^{ab}/\mathbb{Q}) \cong \hat{\mathbb{Z}}^*$, where $\hat{\mathbb{Z}}^* = \mathbb{A}_f^*/\mathbb{Q}_+^*$. In general, for other number fields, one has the "class field theory isomorphism"

$$\theta : \mathrm{Gal}(\mathbb{K}^{ab}/\mathbb{K}) \xrightarrow{\cong} C_{\mathbb{K}}/D_{\mathbb{K}}$$

where $C_{\mathbb{K}} = \mathbb{A}_{\mathbb{K}}^*/\mathbb{K}^*$ is the group of idele classes and $D_{\mathbb{K}}$ the connected component of the identity in $C_{\mathbb{K}}$. In general, however, one does not have an explicit description of the generators of the maximal abelian extension $\mathbb{K}^{ab}$ and the action of the Galois group. This is the content of the explicit class field theory problem, Hilbert's 12th problem. In addition to the Kronecker–Weber case, a complete answer is known in the case of imaginary quadratic fields $\mathbb{K} = \mathbb{Q}(\sqrt{-d})$, with $d > 1$ a positive integer. In this case generators are obtained by evaluating modular functions at a point τ in the upper-half plane such that $\mathbb{K} = \mathbb{Q}(\tau)$ and the Galois action is described explicitly through the group of automorphisms of the modular field, through Shimura reciprocity. For a survey of the explicit class field theory problem and the case of imaginary quadratic fields, see Stevenhagen (2001).

As we mentioned above, understanding the structure of the absolute Galois group $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ is a fundamental question in number theory. Grothendieck described, in his famous proposal "Esquisse d'un programme," how to obtain an action of $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ on an essentially combinatorial object, the set of "dessins d'enfants." These are connected graphs (on a surface) such that the complement of the graph is a union of open cells and the vertices have two different markings, with the properties that adjacent vertices have opposite markings. Such objects arise by considering the projective line $\mathbb{P}^1$ minus three points. Any finite cover of $\mathbb{P}^1$ branched only over $\{0, 1, \infty\}$ gives an algebraic curve defined over $\bar{\mathbb{Q}}$. The dessin is the inverse image under the covering map of the segment $[0, 1]$ in $\mathbb{P}^1$. The absolute Galois group $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ acts on the data of the curve and the covering map, hence on the set of

dessins. A theorem of Bielyi shows that, in fact, all algebraic curves defined over $\bar{\mathbb{Q}}$ are obtained as coverings of the projective line ramified only over the points $\{0, 1, \infty\}$. This has the effect of realizing the absolute Galois group as a subgroup of outer automorphisms of the profinite fundamental group of the projective line minus three points. For a general reference on the subject, see Schneps (1994).

A different type of Galois symmetry of great arithmetic significance is "motivic" Galois theory. This will be discussed later in the section dedicated to motives, where we discuss a surprising occurrence in the context of perturbative quantum field theory and renormalization.

Quantum Statistical Mechanics and Class Field Theory

In quantum statistical mechanics, one considers an algebra of observables, which is a unital C^*-algebra $\mathcal{A}$ with a time evolution σ_t. States are given by linear functionals $\varphi : \mathcal{A} \to \mathbb{C}$ satisfying $\varphi(1) = 1$ and positivity $\varphi(x^*x) \geq 0$. Equilibrium states φ at inverse temperature β satisfy the Kubo–Martin–Schwinger (KMS) condition, namely, for all $x, y \in \mathcal{A}$ there exists a bounded holomorphic function $F_{x,y}(z)$ on the strip $0 < \Im(z) < \beta$, which extends continuously to the boundary, such that for all $t \in \mathbb{R}$

$$F_{x,y}(t) = \varphi(x\sigma_t(y))$$

and

$$F_{x,y}(t + i\beta) = \varphi(\sigma_t(y)x) \qquad [5]$$

Cases of number-theoretic interest arise when one considers the noncommutative space of commensurability classes of $\mathbb{Q}$-lattices up to scaling as algebra of observables, with a natural time evolution determined by the covolume, as shown in the paper *Quantum Statistical Mechanics of $\mathbb{Q}$-Lattices* of Connes–Marcolli (Julia *et al.* 2005, vol. I). A $\mathbb{Q}$-lattice in $\mathbb{R}^n$ consists of a pair (Λ, ϕ) of a lattice $\Lambda \subset \mathbb{R}^n$ together with a homomorphism of abelian groups $\phi : \mathbb{Q}^n/\mathbb{Z}^n \longrightarrow \mathbb{Q}\Lambda/\Lambda$. Two $\mathbb{Q}$-lattices are commensurable, $(\Lambda_1, \phi_1) \sim (\Lambda_2, \phi_2)$, iff $\mathbb{Q}\Lambda_1 = \mathbb{Q}\Lambda_2$ and $\phi_1 = \phi_2 \bmod \Lambda_1 + \Lambda_2$.

The Bost–Connes system The quantum statistical mechanical system considered by Bost and Connes (1995) corresponds to the case of one-dimensional $\mathbb{Q}$-lattices. The partition function of the system is the Riemann zeta function $\zeta(\beta)$. The system has spontaneous symmetry breaking at $\beta = 1$, with a single KMS state for all $0 < \beta \leq 1$. For $\beta > 1$, the extremal equilibrium states are parametrized by the embeddings of $\mathbb{Q}^{\mathrm{cycl}}$ in $\mathbb{C}$ with a free transitive action of the idele class group $C_{\mathbb{Q}}/D_{\mathbb{Q}} = \hat{\mathbb{Z}}^*$. At zero temperature, the evaluation of KMS_∞ states on elements of a rational subalgebra intertwines the action of $\hat{\mathbb{Z}}^*$ by automorphisms of $(\mathcal{A}, \sigma_t)$ with the action of $\mathrm{Gal}(\mathbb{Q}^{ab}/\mathbb{Q})$ on the values of the states. This recovers the explicit class field theory of $\mathbb{Q}$ from a physical perspective.

Noncommutative space of adele classes The algebra $\mathcal{A}$ of the Bost–Connes system is the noncommutative algebra of functions $f(r, \rho)$, for $\rho \in \hat{\mathbb{Z}}$ and $r \in \mathbb{Q}^*$ such that $r\rho \in \hat{\mathbb{Z}}$, with the convolution product

$$f_1 * f_2(r, \rho) = \sum_{s \in \mathbb{Q}^* : s\rho \in \hat{\mathbb{Z}}} f_1(rs^{-1}, s\rho) f_2(s, \rho) \qquad [6]$$

and the adjoint $f^*(r, \rho) = \overline{f(r^{-1}, r\rho)}$. According to the general philosophy of Connes style noncommutative geometry, it is the algebra of coordinates of the noncommutative space defined by the "bad quotient" $\mathrm{GL}_1(\mathbb{Q}) \backslash (\mathbb{A}_f \times \{\pm 1\})$ – a noncommutative version of the zero-dimensional Shimura variety $\mathrm{Sh}(\mathrm{GL}_1, \{\pm 1\}) = \mathrm{GL}_1(\mathbb{Q}) \backslash (\mathrm{GL}_1(\mathbb{A}_f) \times \{\pm 1\})$. Its "dual system" (in the sense of Connes's duality of type III and type II factors) is obtained by taking the crossed product by the time evolution. It gives the algebra of coordinates of the noncommutative space defined by the quotient $\mathbb{A}/\mathbb{Q}^*$. This is the noncommutative space of "adele classes" used by Connes in his spectral realization of the zeros of the Riemann zeta function.

The GL_2-system A generalization of the Bost–Connes system was introduced by Connes and Marcolli in the paper *Quantum Statistical Mechanics of $\mathbb{Q}$-Lattices* (Julia *et al.* 2005). This corresponds to the case of two-dimensional $\mathbb{Q}$-lattices. The partition function is the product $\zeta(\beta)\zeta(\beta - 1)$. The system in this case has two phase transitions, with no KMS states for $\beta \leq 1$. For $\beta > 2$, the extremal KMS states are parametrized by the invertible $\mathbb{Q}$-lattices, namely, those for which ϕ is an isomorphism. The algebra $\mathcal{A}$ has an arithmetic structure given by a rational algebra of unbounded multipliers. This rational algebra contains modular functions and Hecke operators. At zero temperature, extremal KMS states can be evaluated on these multipliers. Symmetries of $(\mathcal{A}, \sigma_t)$ are realized in part by endomorphisms (as in the theory of superselection sectors) and the symmetry group acting on low-temperature KMS states is the group of automorphisms of the modular field $\mathrm{GL}_2(\mathbb{A}_f)/\mathbb{Q}^*$. For a generic set of extremal KMS_∞ states, evaluation at the rational algebra intertwines this action with the action on the values of an embedding of the modular field as a subfield of $\mathbb{C}$.

The complex multiplication system In the case of an imaginary quadratic field $\mathbb{K} = \mathbb{Q}(\tau)$, an analogous construction is possible. A one-dimensional $\mathbb{K}$-lattice is a pair (Λ, ϕ) of a finitely generated $\mathcal{O}$-submodule Λ of $\mathbb{C}$, with $\Lambda\mathbb{K} = \mathbb{K}$, and a homomorphism of $\mathcal{O}$-modules $\phi : \mathbb{K}/\mathcal{O} \to \mathbb{K}\Lambda/\Lambda$. Two $\mathbb{K}$-lattices are commensurable iff $\mathbb{K}\Lambda_1 = \mathbb{K}\Lambda_2$ and $\phi_1 = \phi_2 \bmod \Lambda_1 + \Lambda_2$. Connes *et al.* (Preprint 2005) constructed a quantum statistical mechanical system describing the noncommutative space of commensurability classes of one-dimensional $\mathbb{K}$-lattices up to scale. The partition function is the Dedekind zeta function $\zeta_{\mathbb{K}}(\beta)$. The system has a phase transition at $\beta = 1$ with a unique KMS state for higher temperatures and extremal KMS states parametrized by the invertible $\mathbb{K}$-lattices at lower temperatures. There is a rational subalgebra induced by the rational structure of the GL_2-system (one-dimensional $\mathbb{K}$-lattices are also two-dimensional $\mathbb{Q}$-lattices with compatible notions of commensurability). The symmetries of the system are given by the idele class group $\mathbb{A}^*_{\mathbb{K},f}/\mathbb{K}^*$. The action is partly realized by endomorphisms corresponding to the possible presence of a nontrivial class group (for class number >1). The values of extremal KMS_∞ states on the rational subalgebra intertwine the action of the idele class group with the Galois action on the values. This fully recovers the explicit class field theory for imaginary quadratic fields.

Conformal Field Theory and the Absolute Galois Group

Moore and Seiberg considered data associated to any rational conformal field theory, consisting of matrices, obtained as monodromies of some holomorphic multivalued functions on the relevant moduli spaces, satisfying polynomial equations. Under reasonable hypotheses, the coefficients of the Moore–Seiberg matrices are algebraic numbers. This allows for the presence of interesting arithmetic phenomena. Through the Chern–Simons/Wess–Zumino–Witten correspondence, it is possible to construct three-dimensional topological field theories from solutions to the Moore–Seiberg equations.

On the arithmetic side, Grothendieck proposed in his "Esquisse d'un programme" the existence of a Teichmüller tower given by the moduli spaces $M_{g,n}$ of Riemann surfaces of arbitrary genus g and number of marked points n, with maps defined by operations such as cutting and pasting of surfaces and forgetting marked points, all encoded in a family of fundamental groupoids. He conjectured that the whole tower can be reconstructed from the first two levels, providing, respectively, generators and relations. He called this a "game of Lego–Teichmüller." He also conjectured that the absolute Galois group acts by outer automorphisms on the profinite completion of the tower. The basic building blocks of the tower are provided by "pairs of pants," that is, by projective lines minus three points.

This leads to a conjectural relation between the Moore–Seiberg equations and this Grothendieck–Teichmüller setting (cf. Degiovanni 1994) according to which solutions of the Moore–Seiberg equations provide projective representations of the Teichmüller tower, and the action of the absolute Galois group $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ corresponds to the action on the coefficients of the Moore–Seiberg matrices.

Rational conformal field theories are, in general, one of the most promising sources of interactions between number theory and physics, involving interesting Galois actions, modular forms, Brauer groups, and complex multiplication. Some fundamental work in this direction was done by, for example, Borcherds and Gannon.

Arithmetic Algebraic Geometry

In this section we describe occurrences in physics of various aspects of the arithmetic geometry of algebraic varieties.

Arithmetic Calabi–Yau

In the context of type II string theory, compactified on Calabi–Yau 3-folds, Greg Moore considered certain black hole solutions and a resulting dynamical system given by a differential equation in the corresponding moduli. The fixed points of these equations determine certain "black hole attractor varieties." In the case of varieties obtained from a product of elliptic curves or of a K3 surface and an elliptic curve, the attractor equation singles out an arithmetic property: the elliptic curves have complex multiplication. The class number of the corresponding imaginary quadratic field counts U-duality classes of black holes with the same area. Other results point to a relation between the arithmetic properties of Calabi–Yau 3-folds and conformal field theory. For instance, it was shown by Schimmrigk that, in certain cases, the algebraic number field defined via the fusion rules of a conformal field theory as the field defined by the eigenvalues of the integer-valued fusion matrices

$$\phi_i * \phi_j = (N_i)_j^k \phi_k$$

can be recovered from the Hasse–Weil L-function of the Calabi–Yau. An interesting case is provided by the Gepner model associated with the Fermat quintic Calabi–Yau 3-fold.

Arakelov Geometry

For $\mathbb{K}$ a number field and $O_{\mathbb{K}}$ its ring of integers, a smooth proper algebraic curve X over $\mathbb{K}$ determines a smooth minimal model $X_{O_{\mathbb{K}}}$, which defines an arithmetic surface $\mathcal{X}_{O_{\mathbb{K}}}$ over $\mathrm{Spec}(O_{\mathbb{K}})$. The closed fiber $X_{\wp}$ of $\mathcal{X}_{O_{\mathbb{K}}}$ over a prime $\wp \in O_{\mathbb{K}}$ is given by the reduction mod $\wp$.

When $\mathrm{Spec}(O_{\mathbb{K}})$ is "compactified" by adding the Archimedean primes, one can correspondingly enlarge the group of divisors on the arithmetic surface by adding formal real linear combinations of irreducible "closed vertical fibers at infinity." Such fibers are only treated as formal objects. The main idea of Arakelov geometry is that it is sufficient to work with "infinitesimal neighborhood" $X_\alpha(\mathbb{C})$ of these fibers, given by the Riemann surfaces obtained from the equation defining X over $\mathbb{K}$ under the embeddings $\alpha: \mathbb{K} \hookrightarrow \mathbb{C}$ that constitute the Archimedean primes. Arakelov developed a consistent intersection theory on arithmetic surfaces, by computing the contribution of the Archimedean primes to the intersection indices using Hermitian metrics on these Riemann surfaces and the Green function of the Laplacian.

A general introduction to the subject of Arakelov geometry can be found in Lang (1988). Manin (1991) showed that these Green functions can be computed in terms of geodesics in a hyperbolic 3-manifold that has the Riemann surface $X_\alpha(\mathbb{C})$ as its conformal boundary at infinity.

The Polyakov measure A first application to physics of methods of Arakelov geometry was an explicit formula obtained by Beilinson and Manin (1986) for the Polyakov bosonic string measure in terms of Faltings's height function at algebraic points of the moduli space of curves.

The partition function for the closed bosonic string has a perturbative expansion $Z = \sum_{g \geq 0} Z_g$, with

$$Z_g = \mathrm{e}^{\beta(2-2g)} \int_\Sigma \mathrm{e}^{-S(x,\gamma)} DxD\gamma \qquad [7]$$

written in terms of a compact Riemann surface Σ of genus g, maps $x: \Sigma \to \mathbb{R}^d$, and metrics γ on Σ. The classical action is of the form

$$S(x,\gamma) = \int_\Sigma \mathrm{d}^2 z \sqrt{|\gamma|}\gamma^{ab}\partial_a x^\mu \partial_b x^\mu \qquad [8]$$

Using the invariance of the classical action with respect to the semidirect product of diffeomorphisms of Σ and the conformal group, the integral is reduced (in the critical dimension $d = 26$ where the conformal anomaly cancels) to a zeta regularized determinant of the Laplacian for the metric on Σ and an integration over the moduli space M_g of genus g algebraic curves. Beilinson and Manin gave an explicit formula for the resulting Polyakov measure on M_g using results of Faltings on Arakelov geometry of arithmetic surfaces. In particular, their argument uses essentially the properties of the Faltings metrics on the invertible sheaves $d(L)$ given by the "multiplicative Euler characteristics" of sheaves L of relative 1-forms. For a suitable choice of bases $\{\phi_j\}$ and $\{w_j\}$ of differentials and quadratic differentials, the formula for the Polyakov measure is then of the form (up to a multiplicative constant)

$$\mathrm{d}\pi_g = |\det B|^{-18}(\det \Im\tau)^{-13} W_1 \wedge \bar{W}_1 \wedge \cdots \wedge W_{3g-3} \wedge \bar{W}_{3g-3} \qquad [9]$$

with τ in the Siegel upper-half space, $B_{ij} = \int_{a_i} \phi_j$, and the W_j given by the images of the basis w_j under the Kodaira–Spencer isomorphism.

Holography In the case of the elliptic curve $X_q(\mathbb{C}) = \mathbb{C}^*/q^{\mathbb{Z}}$, a formula of Alvarez-Gaume, Moore, and Vafa gives the operator product expansion of the path integral for bosonic field theory as

$$g(z,1) = \log\left(|q|^{B_2(\log|z|/\log|q|)/2}|1-z| \times \prod_{n=1}^{\infty} |1-q^n z|\,|1-q^n z^{-1}| \right) \qquad [10]$$

where B_2 is the second Bernoulli polynomial. Expression [8] is in fact the Arakelov Green function on $X_q(\mathbb{C})$ (cf. Lang (1988)).

Using this and analogous results for higher genus Riemann surfaces, Manin and Marcolli (2001) showed that the result of Manin (1991) on Arakelov and hyperbolic geometry can be rephrased in terms of the AdS/CFT correspondence, or holography principle. Expression [8] can then be written as a combination of terms involving geodesic lengths in the Euclidean BTZ black hole.

In the case of higher genus curves, the Arakelov Green function on a compact Riemann surface, which is related to the two-point correlation function for bosonic field theory, can be expressed in terms of the semiclassical limit of gravity (the geodesic propagator) on the bulk space of Euclidean versions of asymptotically AdS_{2+1} black holes introduced by K Krasnov.

Motives

There are several cohomology theories for algebraic varieties: de Rham, Betti, étale cohomology. de Rham

and Betti are related by the period isomorphism, and comparison isomorphisms relate Étale and Betti cohomology. In the smooth projective case, they have the expected properties of Poincaré duality, Künneth isomorphisms, etc. Moreover, Étale cohomology provides interesting ℓ-adic representations of $\mathrm{Gal}(\bar{k}/k)$. In order to understand what type of information, such as maps or operations can be transferred from one to another cohomology, Grothendieck introduced the idea of the existence of a "universal cohomology theory" with realization functors to all the known cohomology theories for algebraic varieties. He called this the theory of "motives." Properties that can be transferred between different cohomology theories are those that exist at the motivic level. A short introduction to motives can be found in Serre (1992).

The first constructions of a category of motives proposed by Grothendieck covers the case of smooth projective varieties. The corresponding motives form a $\mathbb{Q}$-linear abelian category of "pure motives." Roughly, objects are varieties and morphisms are "correspondences" given by algebraic cycles in the product, modulo a suitable equivalence relation. The category also contains Tate objects generated by $\mathbb{Q}(1)$, which is the inverse of the pure motive $H^2(\mathbb{P}^1)$. Grothendieck's standard conjectures imply that the category of pure motives is equivalent to the category of representations Rep_G of a "motivic Galois group," which in the case of pure motives is proreductive. The subcategory of pure Tate motives has as motivic Galois group the multiplicative group $\mathbb{G}_m$. The situation is more complicated for "mixed motives," for which constructions were only very recently proposed (e.g., in the work of Voevodsky). These provide a universal cohomology theory for more general classes of algebraic varieties. Mixed Tate motives are the subcategory generated by the Tate objects. There is again a motivic Galois group. For mixed motives it is an extension of a proreductive group by a prounipotent group, with the proreductive part coming from pure motives and the prounipotent part from the presence of a weight filtration on mixed motives. The multiple zeta values appear as periods of mixed Tate motives.

Renormalization and Motivic Galois Theory

A manifestation of motivic Galois groups in physics arises in the context of the Connes–Kreimer theory of perturbative renormalization (for an introduction to this topic, *see* Hopf Algebra Structure of Renormalizable Quantum Field Theory). In fact, according to the Connes–Kreimer theory, the Bogoliubov–Parasiuk–Hepp–Zimmerman (BPHZ) renormalization scheme with dimensional regularization and minimal subtraction can be formulated mathematically in terms of the Birkhoff factorization

$$\gamma(z) = \gamma_-(z)^{-1}\gamma_+(z) \qquad [11]$$

of loops in a prounipotent Lie group G, which is the group of characters of the Hopf algebra of Feynman graphs. Here, the loop γ is defined on a small punctured disk around the critical dimension D, γ_+ is holomorphic in a neighborhood of D, and γ_- is holomorphic in the complement of D in $\mathbb{P}^1(\mathbb{C})$. The renormalized value is given by $\gamma_+(D)$ and the counterterms by $\gamma_-(z)$.

The paper of Connes and Marcolli *Renormalization, the Riemann–Hilbert Correspondence*, and *Motivic Galois Theory* in volume II of Julia *et al.* (2005) shows that the data of the Birkhoff factorization are equivalently described in terms of solutions to a certain class of differential systems with irregular singularities. This is obtained by writing the terms in the Birkhoff factorization as time-ordered exponentials, and then using the fact that

$$\mathrm{T}e^{\int_a^b \alpha(t)\,dt} := 1 + \sum_{n=1}^{\infty} \int_{a\le s_1\le\cdots\le s_n\le b} \alpha(s_1)\cdots\alpha(s_n)\,ds_1\cdots ds_n$$

is the value $g(b)$ at b of the unique solution $g(t) \in G$ with value $g(a) = 1$ of the differential equation $dg(t) = g(t)\alpha(t)\,dt$.

The singularity types are specified by physical conditions, such as the independence of the counterterms on the mass scale. These conditions are expressed geometrically through the notion of G-valued "equisingular connections" on a principal $\mathbb{C}^*$-bundle B over a disk Δ, where G is the prounipotent Lie group of characters of the Connes–Kreimer Hopf algebra of Feynman graphs. The "equisingularity" condition is the property that such a connection ω is $\mathbb{C}^*$-invariant and that its restrictions to sections of the principal bundle that agree at $0 \in \Delta$ are mutually equivalent, in the sense that they are related by a gauge transformation by a G-valued $\mathbb{C}^*$-invariant map regular in B; hence, they have the same type of (irregular) singularity at the origin.

The classification of equivalence classes of these differential systems via the Riemann–Hilbert correspondence and differential Galois theory yields a Galois group $U^* = U \rtimes \mathbb{G}_m$, where U is prounipotent, with Lie algebra the free graded Lie algebra with one generator e_{-n} in each degree $n \in \mathbb{N}$. The group U^* is identified with the motivic Galois group of mixed Tate motives over the cyclotomic ring $\mathbb{Z}[e^{2\pi i/N}]$, for $N = 3$ or $N = 4$, localized at N.

Speculations on Arithmetical Physics

In a lecture written for the 25th Arbeitstagung in Bonn, Y Manin presented intriguing connections between arithmetic geometry (especially Arakelov geometry) and physics. The theme is also discussed in Manin (1989). These considerations are based on a philosophical viewpoint according to which fundamental physics might, like adeles, have Archimedean (real or complex) as well as non-Archimedean (p-adic) manifestations. Since adelic objects are more fundamental and often simpler than their Archimedean components, one can hope to use this point of view in order to carry over some computation of physical relevance to the non-Archimedean side where one can employ number-theoretic methods.

Adelic physics? Some of the results mentioned in the previous sections seem to lend themselves well to this adelic interpretation. The quantum statistical mechanics of $\mathbb{Q}$-lattices relies fundamentally on adeles and it admits generalizations to systems associated to other algebraic varieties (Shimura varieties) that have an adelic description and adelic groups of symmetries. The result on the Polyakov measure also has an adelic flavor, as it uses essentially the Archimedean component of the Faltings height function. The latter is in fact a product of contributions from all the Archimedean and non-Archimedean places of the field of definition of algebraic points in the moduli space, so that one can expect that there would be an adelic Polyakov measure, of which one normally sees the Archimedean side only. The Freund–Witten adelic product formula for the Veneziano string amplitude fits in the same context, with p-adic amplitudes

$$B_p(\alpha, \beta) = \int_{\mathbb{Q}_p} |x|_p^{\alpha-1} |1-x|_p^{\beta-1}\, dx$$

and $B_\infty(\alpha, \beta)^{-1} = \prod_p B_p(\alpha, \beta)$ (cf. Varadarajan (2004)).

Adelic physics and motives A similar adelic philosophy was taken up by other authors, who proposed ways of introducing non-Archimedean and adelic geometries in quantum physics. A recent survey is given in Varadarajan (2004). For instance, Volovich (1995) proposed spacetime models based on cohomological realizations of motives, with étale topology "interpolating" between a proposed non-Archimedean geometry at the Planck scale and Euclidean geometry at the macroscopic scale. In this viewpoint, motivic L-functions appear as partition functions and actions of motivic Galois groups govern the dynamics.

See also: Hopf Algebra Structure of Renormalizable Quantum Field Theory; Mirror Symmetry: A Geometric Survey; Quantum Ergodicity and Mixing of Eigenfunctions; Random Matrix Theory in Physics; Regularization for Dynamical Zeta Functions.

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O

Operads

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Introduction

An operad is an abstraction of a family of composable functions of n variables for various n, useful for the "bookkeeping" and applications of such families. Operads are particularly important and useful in categories with a good notion of "homotopy," where they play a key role in organizing hierarchies of higher homotopies, reflecting their original use as a tool in homotopy theory, especially for studying (iterated) loop spaces. For several years now, operads have become increasingly important in mathematical physics, especially in string field theory, where they organize the terms of higher order in perturbed actions, and in deformation quantization.

The major focus of this article will be on operads as they are relevant to mathematical physics, but will also include some background material from homotopy theory, where they originated. A borderland where homotopy theory and cohomological physics overlap is the world of differential graded vector spaces, including those of differential forms, ghosts, anti-ghosts, etc., sometimes lumped together as BRST theory. Here, as elsewhere in contemporary mathematical physics, the flow has been in both directions – sometimes physicists have discovered or reinvented known mathematics but finding new applications, at other times physics has suggested new concepts for mathematicians to develop further. In the case of operads, they have provided general structure for varieties of algebras, some of which are novel types contributed by physicists.

For a reasonably up-to-date introduction and survey, consider Markl *et al.* (2002), although there have been many developments since then. Two particularly important original works are Boardman and Vogt (1973) and May (1972).

Definitions and Examples

The term "operad" is due to May, building on work of Stasheff and of Boardman–Vogt. The most fundamental example of an operad is the endomorphism operad $\mathcal{E}nd_X := \{\mathrm{Map}(X^n, X)\}_{n \geq 1}$ where, for a set or topological space X, $\{\mathrm{Map}(X^n, X)\}$ means the set or space of functions or continuous functions from the n-fold product of X with itself to X, together with the operations

$$\circ_i : Map(X^n, X) \times Map(X^m, X) \longrightarrow Map(X^{n+m-1}, X)$$

given, for $1 \leq i \leq n$, by

$$(f \circ_i g)(x_1, \ldots, x_{m+n-1}) \\ = f(x_1, \ldots, x_{i-1}, g(x_i, \ldots, x_{i+m-1}), x_{i+m}, \ldots)$$

In the endomorphism operad $\mathcal{E}nd_X$, there are easily discovered relations involving iterated $\circ_i$-operations and the symmetric group Σ_n actions on the X^ns. For example,

$$(f \circ_i g) \circ_j h = f \circ_i (g \circ_{j-i+1} h) \\ \text{for } i \leq j \leq i + m - 1$$

if g is a function of m variables, since only the name of the position for the insertion is changed.

An operad $(\mathcal{O}, \circ_i)$ consists of a collection $\{\mathcal{O}(n)\}_{n \geq 1}$ of objects and maps $\circ_i : \mathcal{O}(n) \times \mathcal{O}(m) \rightarrow \mathcal{O}(n + m - 1)$ for $m, n \geq 1$ and $i \leq n$ satisfying the relations manifest in the example $\mathcal{E}nd_X$.

May's original definition corresponds to simultaneous insertions into all possible positions of inputs into $f \in Map(X^n, X)$. In most examples, the structures are "manifest" without appeal to the technical definitions.

It helps to see graphic examples of operads, particularly ones relevant for physics. Two kinds that are particularly important are the tree operads and the little disks (or cubes) operads.

Let $\mathcal{T}(n)$ be the set of planar trees with one root and n leaves labeled (arbitrarily) 1 through n. The collection $\mathcal{T} = \{\mathcal{T}(n)\}_{n \geq 1}$ of sets of trees forms an operad by grafting the root of g to the leaf of f labeled i, as in **Figure 1**, where the leaves are assumed labeled in order from left to right. **Figure 1** can be interpreted as portraying the $\circ_4$ result of inserting a 3-linear operation into a 5-linear one.

The little n-disks operad $\mathcal{D}_n = \{\mathcal{D}_n(j)\}_{j \geq 1}$ where $\mathcal{D}_n(j)$ consists of an ordered collection of j n-disks

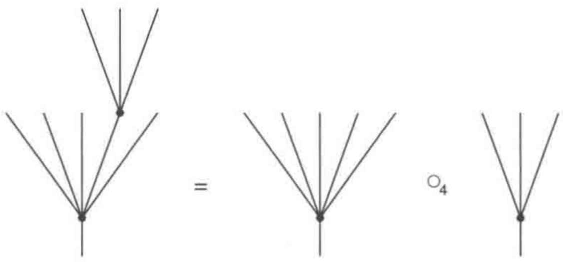


Figure 1 Grafting with the leaves numbered from left to right.

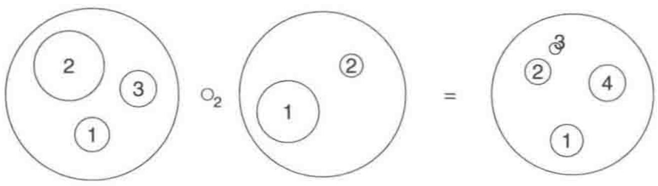


Figure 2 The little 2-disks operad.

embedded in the standard n-dimensional unit disk D^n with disjoint interiors, the embedding being of the form $az + b$ with $0 < a \in \mathbb{R}$. The operations are given as indicated in **Figure 2**.

Just as group theory without representations is rather sterile, so are operads best appreciated by their representations known as (varieties of) algebras, especially algebras with higher homotopies.

An algebra A over an operad $\mathfrak{P}$ "is" a map of operad $\mathfrak{P} \to \mathcal{E}nd_A$. This is just a compact way of saying that an algebra A has a coherent system of maps $\mathfrak{P}(n) \times A^n \to A$. Much of this article will speak in terms of such algebras with the corresponding operad being understood.

Operads in Homotopy Theory

A major motivation for the development of operads was the desire to have a homotopy-invariant characterization of based loop spaces and iterated loop spaces. Precisely such coherent systems of higher homotopies provided the answers. For based loop spaces, the operad in question $\mathcal{K} = \{K_n\}_{n \geq 1}$ consists of the polytopes known as "associahedra." The usual product of based loops is only homotopy associative.

If we fix a specific associating homotopy and consider the five ways of parenthesizing the product of four loops, there results a pentagon whose edges correspond to a path of loops (**Figure 3**).

From the leftmost vertex to the rightmost, consider the two paths of loops across the top or around the bottom. By further adjustment of parameters, the pentagon can be filled in by a family of such paths.

The associahedron K_n can be described as a convex polytope with one vertex for each way of associating n ordered variables, that is, ways of inserting parentheses in a meaningful way in a word

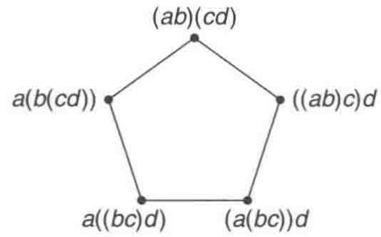


Figure 3 The associahedron K_4.

of n letters. The edges correspond to a single application of an associating homotopy. More generally, the cellular structure of the associahedra is well described by planar rooted trees, the vertices corresponding to binary trees and so forth (see **Figure 4**).

For K_5, see **Figure 5** or a rotatable image available at http://igd.univ-lyon1.fr/~ chapoton/stasheff.html. The facets are all products of two associahedra of lower dimension and specific imbeddings can be given to play the role of the $\circ_i$ operations as in an operad.

An A_∞-space is a space Y which admits a coherent family of maps

$$m_n : K_n \times Y^n \to Y$$

so that they make Y an algebra over the operad (without Σ_n-actions) $\mathcal{K} = \{K_n\}_{n \geq 1}$.

The main result by Stasheff is: A connected space Y (of the homotopy type of a CW-complex) has the homotopy type of a based loop space ΩX for some X if and only if Y is an A_∞-space.

Homotopy characterization of iterated loop spaces $\Omega^n X_n$ for some space X_n required the full power of the theory of operads with the symmetries.

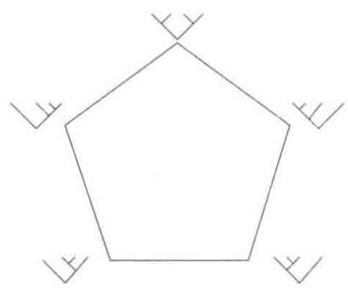


Figure 4 K_4 with vertices labeled by trees.

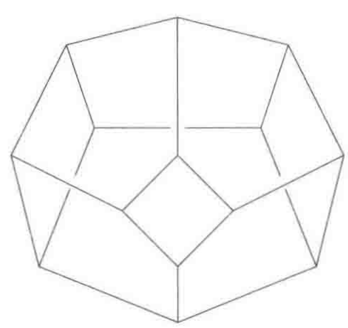


Figure 5 The associahedron K_5.

An early motivation for the invention of a theory of operads was the consideration of infinite loop spaces, that is, a sequence of spaces X_n such that each X_n is homotopy equivalent to ΩX_{n+1}.

Although introduced originally in the category of topological spaces, operads were available almost immediately for differential graded (dg) vector spaces, also known as chain complexes. In physics, the differential is often called a BRST operator, a term that should be reserved for a special kind of dg algebra, see below.

Operads in Algebra

The $\circ_i$ notation first appeared in Gerstenhaber's study of the algebraic structure of the Hochschild cohomology of an associative algebra, about the same time as the construction of the associahedra where the operations were given in a less convenient notation. Recall the Hochschild cohomology of an associative algebra A is the homology of the complex $\mathrm{Hom}(A^{\otimes n}, A)$ with the coboundary given as follows (all signs below are indicated as $\pm$, any of the standard references will specify conventions and signs): for $f \in \mathrm{Hom}(A^{\otimes n}, A)$ and $g \in \mathrm{Hom}(A^{\otimes m}, A)$ let

$$f \circ g = \Sigma_1^n \pm f \circ_i g \qquad [1]$$

Gerstenhaber then defines his bracket as $[f, g] = f \circ g \pm g \circ f$. With hindsight, he realized that the Hochschild coboundary can be written as

$$\delta h = [m, h] \qquad [2]$$

where $m: A \otimes A \to A$ is the multiplication. Moreover, the associativity of m is equivalent to

$$[m, m] = 0 \qquad [3]$$

A_∞-Algebras

In the setting of graded vector spaces $V = \oplus_{r \in \mathbb{Z}} V^r$, there are two conventions for defining A_∞-algebras, which differ by a shift in grading. We adopt the physics convention so that A here is the suspension of that considered in the original papers. The cellular chains of the associahedra form the A_∞-operad, providing the following definition.

Definition 1 A_∞-algebra (Strong homotopy associative algebra). Let A be a $\mathbb{Z}$-graded vector space $A = \oplus_{r \in \mathbb{Z}} A^r$ and suppose that there exists a collection of degree 1 multilinear maps

$$\mathfrak{m} := \{m_k : A^{\otimes k} \to A\}_{k \geq 1}$$

$(A, \mathfrak{m})$ is called an A_∞-algebra when the multilinear maps m_k satisfy the following relations:

$$\sum_{p+q=n+1} \sum_{i=1}^{p} \pm m_p \circ_i m_q = 0 \qquad [4]$$

with an appropriate set of signs for $n \geq 1$.

A weak A_∞-algebra consists of a collection of degree 1 multilinear maps

$$\mathfrak{m} := \{m_k : A^{\otimes k} \to A\}_{k \geq 0}$$

satisfying the above relations, but for $n \geq 0$ and in particular with $k, l \geq 0$.

Remark 1 The "weak" version is fairly new, inspired by physics, where $m_0: \mathbb{C} \to A$, regarded as an element $m_0(1) \in A$, is related to what physicists refer to as a "background." The augmented relation then implies that $m_0(1)$ is a cycle, but $m_1 m_1$ need no longer be 0, rather

$$m_1 m_1 = \pm\, m_2(m_0 \otimes 1) \pm\, m_2(1 \otimes m_0) \qquad [5]$$

Just as associativity was captured by the equation $[m, m] = 0$, so the defining relations of the definition of an A_∞-algebra are captured by

$$[\mathfrak{m}, \mathfrak{m}] = 0 \qquad [6]$$

Decades later it was realized that considering $T^c A = \Sigma A^{\otimes n}$ as a coalgebra with

$$\Delta(a_1 \otimes \cdots \otimes a_n) = \Sigma_{p+q} \pm (a_1 \otimes \cdots \otimes a_p) \otimes (a_{p+1} \otimes \cdots \otimes a_n)$$

we then have an isomorphism

$$\Sigma \mathrm{Hom}(A^{\otimes n}, A) \simeq \mathrm{Coder}(T^c A)$$

Here Coder is the space of all coderivations of $T^c A$. The Gerstenhaber bracket is indeed the "intrinsic" commutator bracket of coderivations via the above isomorphism. As such, it satisfies a graded version of the Jacobi identity; after a shift in grading from the original one of Hochschild, the Hochschild cochain complex forms a dg Lie algebra.

L_∞-Algebras

Since an ordinary Lie algebra $\mathfrak{g}$ is regarded as ungraded, the defining bracket is regarded as skew-symmetric. For dg Lie algebras and L_∞-algebras, we need graded symmetry, which refers to symmetry with signs determined by the grading. The basic operation is

$$\tau : x \otimes y \mapsto (-1)^{|x||y|} y \otimes x \qquad [7]$$

Also we adopt the convention that tensor products of graded functions or operators have the signs built

in; for example, $(f \otimes g)(x \otimes y) = (-1)^{|g||x|} f(x) \otimes g(y)$. By decomposing each permutation as a product of transpositions, there is then defined the sign of a permutation of n graded elements, for example, for any $c_i \in V, 1 \leq i \leq n$, and any $\sigma \in \mathfrak{S}_n$, the permutation of n graded elements is defined by

$$\sigma(c_1, \ldots, c_n) = (-1)^{\epsilon(\sigma)}(c_{\sigma(1)}, \ldots, c_{\sigma(n)}) \qquad [8]$$

The sign $(-1)^{\epsilon(\sigma)}$ is often referred to as the Koszul sign of the permutation.

Definition 2 (Graded symmetry). A graded symmetric multilinear map of a graded vector space V to itself is a linear map $f: V^{\otimes n} \to V$ such that for any $c_i \in V, 1 \leq i \leq n$, and any $\sigma \in \mathfrak{S}_n$ (the permutation group of n elements), the relation

$$f(c_1, \ldots, c_n) = (-1)^{\epsilon(\sigma)} f(c_{\sigma(1)}, \ldots, c_{\sigma(n)}) \qquad [9]$$

holds.

Definition 3 By a (k, l)-unshuffle of $c_1, \ldots, c_n$ with $n = k + l$ is meant a permutation σ such that for $i < j \leq k$, we have $\sigma(i) < \sigma(j)$ and similarly for $k < i < j \leq k + l$. We denote the subset of (k, l)-unshuffles in $\mathfrak{S}_{k+l}$ by $\mathfrak{S}_{k,l}$ and by $\mathfrak{S}_{k+l=n}$, the union of the subsets $\mathfrak{S}_{k,l}$ with $k + l = n$. Similarly, a $(k_1, \ldots, k_i)$-unshuffle means a permutation $\sigma \in \mathfrak{S}_n$ with $n = k_1 + \cdots + k_i$ such that the order is preserved within each block of length $k_1, \ldots, k_i$. The subset of $\mathfrak{S}_n$ consisting of all such unshuffles we denote by $\mathfrak{S}_{k_1,\ldots,k_i}$.

Definition 4 L_∞-algebra (Strong homotopy Lie algebra). Let L be a graded vector space and suppose that a collection of degree 1 graded symmetric linear maps $\mathfrak{l} := \{l_k : L^{\otimes k} \to L\}_{k \geq 1}$ is given. $(L, \mathfrak{l})$ is called an L_∞-algebra iff the maps satisfy the following relations:

$$\sum_{\sigma \in \mathfrak{S}_{k+l=n}} (-1)^{\epsilon(\sigma)} l_{1+l}(l_k(c_{\sigma(1)}, \ldots, c_{\sigma(k)}), \\ [c_{\sigma(k+1)}, \ldots, c_{\sigma(n)}) = 0 \qquad [10]$$

for $n \geq 1$.

A weak L_∞-algebra consists of a collection of degree 1 graded symmetric linear maps $\mathfrak{l} := \{l_k : L^{\otimes k} \to L\}_{l \geq 0}$ satisfying the above relations, but for $n \geq 0$ and with $k, l \geq 0$.

Remark 2 The alternate definition in which the summation is over all permutations, rather than just unshuffles, requires the inclusion of appropriate coefficients involving factorials.

Just as an A_∞-algebra can be described as a coderivation of $T^c A$, similarly an L_∞-algebra L can be described as a coderivation on $S^c L$, the symmetric subcoalgebra of $T^c A$.

The operad of Lie algebras was defined rather late, although it was earlier implicit in the work of Fred Cohen. It is defined as the homology $H_{n-1}(\mathrm{Config}(\mathbb{R}^2, n))$ for $n \geq 1$, where $\mathrm{Config}(\mathbb{R}^2, n)$ denotes the configuration space of ordered n-tuples of distinct points in $\mathbb{R}^2$. Equivalently, the configurations can be thought of as the centers of the little 2-disks. The open disks being contractible to their centers, this is a suboperad of the full homology $H_\bullet(\mathcal{D}_2)$.

Just as a Lie algebra is obtained from an associative algebra using the commutator as bracket and, inversely, a Lie algebra gives rise to its universal enveloping associative algebra, an L_∞-algebra can be obtained from an A_∞-algebra by n-variable analogs of commutators and there is a universal enveloping A_∞-algebra of a given L_∞-algebra.

Open–Closed Homotopy Algebras

Open–closed string field theory suggests interaction between an L_∞-algebra $\mathcal{H}_c$ and an A_∞-algebra $\mathcal{H}_o$ including a strong homotopy representation of $\mathcal{H}_c$ on $\mathcal{H}_o$ by strong homotopy derivations. Here is the formal definition:

Definition 5 Let $\mathcal{H} = \mathcal{H}_o \oplus \mathcal{H}_c$ be a graded vector space and $(\mathcal{H}_c, \mathfrak{l})$ be a weak L_∞-algebra. Consider a collection of multilinear maps

$$\mathfrak{n} := \{n_{k,l} : (\mathcal{H}_o)^{\otimes k} \otimes (\mathcal{H}_c)^{\otimes l} \to \mathcal{H}_o\}_{k,l \geq 0}$$

each of which is graded symmetric on $(\mathcal{H}_c)^{\otimes l}$. We denote the collection also by $\mathfrak{n}$. We call $(\mathcal{H}, \mathfrak{n}, \mathfrak{l})$ a (partial) open-closed homotopy algebra (OCHA) when $\mathfrak{n}$ satisfies the following relations (up to some factorial coefficients):

$$0 = \sum_{k,l \geq 0} \sum_{p=0}^{m-k} \sum_{\sigma \in \mathfrak{S}_n} \pm n_{m+1-k,n-l}(o_1, \ldots, o_p, \\ n_{k,l}(o_{p+1}, \ldots, o_{p+k}; c_{\sigma(1)}, \ldots, c_{\sigma(l)}), \\ o_{p+k+1}, \ldots, o_m; c_{\sigma(l+1)}, \ldots, c_{\sigma(n)}) \\ + \sum_{\sigma \in \mathfrak{S}_n} \sum_{l=1}^{n} \pm n_{m,n+1-l}(o_1, \ldots, o_m; \\ l_l(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), c_{\sigma(l+1)}, \ldots, c_{\sigma(n)}) \qquad [11]$$

Other Algebras of Interest

The Hochschild complex also has a graded product (without invoking the shift) known as the cup product. Except for the signs and the grading, the bracket and the product satisfy the Leibniz rule of a Poisson algebra on the cohomology; the result is

axiomatized as a "Gerstenhaber algebra." However, on the cochain complex, the Lie bracket and the associative product are compatible only up to homotopy.

This naturally raises the issue of an operad for strong homotopy Gerstenhaber algebras. The operad $\mathcal{G}$ for Gerstenhaber algebras is the homology of the little disks operad, $H_\bullet(\mathcal{D}_2)$. But now we have choices: in addition to relaxing the Leibniz rule up to homotopy, the bracket could be relaxed to be part of an L_∞-algebra and/or the product could be relaxed to be part of an A_∞-algebra. The choice which is now known as the G_∞-operad is defined in terms of a procedure which works for what are known as quadratic operads, indicating they have generators in $\mathcal{O}(2)$ and relations in $\mathcal{O}(3)$: the corresponding $\mathcal{O}_\infty$ has "dual" relations. For example, this gives the classical Koszul duality between Lie and commutative associative algebras. The $\mathcal{G}_\infty$-operad can also be described as the "minimal model" of $\mathcal{G}$ in the sense of Markl.

Another alternative is to consider just the "brace" operations, originally introduced by Kadeishvili and later independently by Getzler, but described in the Hochschild complex setting by Gerstenhaber–Voronov. Together with the cup product, these determine an operad denoted $\mathcal{HG}$ which acts on the Hochschild complex; there is an operad map from $\mathcal{G}_\infty$ to $\mathcal{HG}$, hence $\mathcal{G}_\infty$ also acts on the Hochschild complex. Finally, Tamarkin showed that $\mathcal{G}_\infty$ is quasi-isomorphic to the dg operad of singular chains on the little disks operad, thus providing one of several proofs of what had been a conjecture by Deligne.

Algebras with invariant inner products $<-,->$ are of considerable importance in mathematics and especially in mathematical physics; invariance means $<a, bc> = <ab, c>$ or $<a, [b,c]> = <[a,b], c>$ in, respectively, the associative or the Lie case (with appropriate signs in the graded case). Using the inner product, n-ary operations $A^{\otimes n} \to A$ can be converted to operations $A^{\otimes n+1} \to \mathrm{C}$ of which we can require cyclic symmetry. To handle such algebras, there is a notion of "cyclic operad." In terms of trees, the transition is to take a rooted tree and then regard the root edge as just another leaf. This point of view corresponds to an essential symmetry for particle interactions.

Operads in Mathematical Physics

One reason for the explosive development of operad theory in the 1990s was the introduction of operadic structures in field theories, for example, conformal field theories (CFTs) and string field theories (SFTs). These operadic structures were directly related to the moduli spaces of Riemann surfaces with punctures or boundaries (or other decorations) in these physical theories.

Two special "higher-homotopy algebras" have been emphasized because they are particularly important in mathematical physics: A_∞ for open-string field theory and L_∞ for closed-string field theory and for deformation quantization. Open–closed string field theory combines A_∞-algebra and L_∞-algebra in a particular way known as an OCHA.

The operad for L_∞-algebras is given a very nice and physically relevant geometric interpretation in terms of a real compactification of the moduli space of Riemann spheres with punctures, while for OCHAs, there is a real compactification of the moduli space of Riemann disks with punctures on the boundary or in the interior (bulk). Thus, this operad can be regarded as obtained from a moduli space of configurations of points (punctures) in the disk by compactifying the moduli spaces by adding boundary strata where two (or more) points (punctures) collide. Points on the boundary strata can be visualized as "bubble trees" of disks and/or spheres, see **Figure 6**. Alternatively, the little disks operad can be regarded as being obtained by "decorating" the points with little disks, while for OCHAs there is also a basic half-disk decorated with little disks in the bulk and little half-disks for the boundary points. The corresponding colored operad is Voronov's "Swiss-cheese operad." "Colored" refers to the fact that disks can be inserted into half-disks but not vice versa. Compare trees with two "colors" of edges with grafts restricted to ones which match colors.

On-Shell versus Off-Shell

In cohomological physics, the "on-shell" states or observables are usually given by the cohomology with respect to an internal differential, which in physics is called the BRST differential or BRST operator, though originally this meant the Chevalley–Eilenberg differential associated to the action of the Lie algebra of

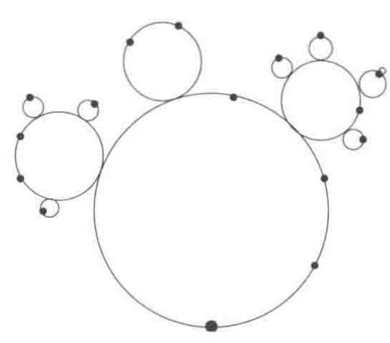


Figure 6 Bubble tree for circle configurations.

gauge symmetries of a physical theory. The generators of the Chevalley–Eilenberg cochain complex are known as "ghosts". On-shell subspaces of algebras which are not closed under the product of the larger "off-shell" algebra are called "open" algebras by physicists. Quite generally, this situation gives rise to an algebra over an appropriate operad. A special case involves a differential graded algebra A and a linear imbedding $H(A) \subset A$. The (co)homology is in turn a graded algebra (with 0 as differential), but inherits a higher-homotopy structure so that cohomology and original algebra are equivalent.

In the associative case, the inheritance is a result of Kadeishvili:

Let (A, d) be a differential graded associative or A_∞-algebra, then the homology $H(A)$ inherits the structure of an A_∞-algebra.

Even if the original algebra A is strictly associative, the inherited A_∞-structure generally has nontrivial operations m_i.

Analogous results hold for L_∞-algebras and others. It is the L_∞-version that is relevant for closed-string field theory (CSFT). Zwiebach showed the quantum theory of covariant closed strings has an action defined in terms of an infinite chain of string field products. The genus-0 (tree level) string field algebra is an L_∞-algebra inherited from the off-shell state space modeled by the Batalin–Vilkovisky (BV) construction. The higher-order brackets provide higher-order correlation or n-point functions which play a crucial role in the extended Lagrangian of the theory.

Batalin–Fradkin–Vilkovisky and Batalin–Vilkovisky Constructions

The constructions of Batalin–Fradkin–Vilkovisky (BFV) for constrained Hamiltonian systems and of Batalin–Vilkovisky (BV) for Lagrangians with symmetries are important examples of L_∞-structures derived from "open" algebra settings, though the L_∞-structures were recognized quite a while after the constructions.

The BFV setting is that of a symplectic manifold W with a family of constraints, that is, a family of functions $\phi^\alpha \in C^\infty(W)$. The constraints are called "first class" if the ideal they generate is closed under the Poisson bracket. The vector space spanned by the constraints will in general be an open algebra; the structure of the bracket is given by structure functions, rather than structure constants. The zero locus of all the constraints forms the constraint surface V. In the first-class case, the constraints are in involution and determine a foliation $\mathcal{F}$ of V. If the space of leaves $V/\mathcal{F}$ is a manifold, it would be considered the true physical space and the physical observables would be functions in $C^\infty(V/\mathcal{F})$. BFV construct a differential graded Poisson algebra such that the cohomology in degree 0 agrees with $C^\infty(V/\mathcal{F})$ when that makes sense and, in the regular case, the rest of the cohomology is that of the differential forms along the leaves of the foliation. The BFV differential is a deformation of the Chevalley–Eilenberg/BRST differential and can be constructed most efficiently by the same techniques used in proving Kadeishivili's inheritance theorem. Crucially, it is an inner derivation with respect to the Poisson bracket. After the fact, an L_∞-structure can be observed in the extended algebra.

For a Lagrangian with symmetries, BV develop a similar construction, the main difference being that there is no Poisson bracket initially, but one is constructed by adjoining "anti-fields" as conjugate to the fields but of ghost degree –1 and the differential of an anti-field being the Euler–Lagrange expression for the corresponding field. Then, as in the Hamiltonian case, ghosts and anti-ghosts, etc. are adjoined and the construction proceeds in a parallel fashion.

Deformation Quantization

Once algebras over an operad $\mathfrak{P}$ are considered, it is natural to consider also morphisms of such algebras over a fixed $\mathfrak{P}$.

From a homotopy point of view, the appropriate maps need not respect the operad structure strictly but only up to higher homotopy; indeed, there is a related operad to define such maps. For L_∞-algebras, such L_∞-maps play a key role in deformation quantization. That refers to deformation of the commutative multiplication of a Poisson algebra in the direction of the Poisson bracket; that is, to first order, the deformation is given by the bracket.

More generally, for any associative algebra A with multiplication m, one considers formal deformations

$$a \star b = m(a, b) + t m_1(a, b) + t^2 m_2(a, b) + \cdots \quad [12]$$

where each $m_i \in \mathrm{Hom}(A \otimes A, A)$. The associativity of $\star$ provides a sequence of constraints on the m_i. In particular, m_1 must be a Hochschild cocycle and the obstruction to the existence of m_2 is a class in the Hochschild cohomology of degree 3. In fact, the primary obstruction is represented by $[m_1, m_1]$. If it is cohomologous to zero, that fact identifies candidates for m_2, that is,

$$[m_1, m_1] = \pm 2[m, m_2] \quad [13]$$

or, using the notation $d = [m,]$,

$$dm_2 - 1/2[m_1, m_1] = 0 \quad [14]$$

once known as the integrability equation but now, more frequently, as a Maurer–Cartan equation. For a Poisson algebra, the Poisson bracket is a Hochschild cocycle but in general a full deformation need not exist. However, for the algebra A of smooth functions on a Poisson (e.g., symplectic) manifold M, Kontsevich showed that such a full formal deformation does exist.

The guiding philosophy is that deformations are controlled by a dg Lie or L_∞-algebra L, unique up to L_∞-homotopy equivalence. Therefore, the obstructions can be computed in any of the equivalent dg Lie algebras. Moreover, the structure of the obstructions is known sufficiently so that if there is an equivalent dg Lie algebra with d in fact zero, then all the obstructions to deformation quantization vanish. The key to Kontsevich's proof was the construction of an L_∞-map, inducing an isomorphism in cohomology, from the Lie algebra of polyvector fields on $\mathbb{R}^d$ with the Schouten bracket and $d=0$ to the Lie algebra of multidifferential operators on $A=C^\infty(\mathbb{R}^d)$ regarded as a subalgebra of the Hochschild cochain complex for A with the Gerstenhaber bracket.

BV Algebras

In addition to their construction of a differential graded Gerstenhaber algebra (a differential graded commutative algebra with a compatible Poisson bracket of degree 1), BV introduced a new mathematical structure, adding a second-order differential operator Δ relating the commutative product and the bracket. The operator Δ is a derivation of the bracket and of square zero. Moreover,

$$[a,b] = \Delta(ab) - \Delta(a)b \pm a\Delta(b) \qquad [15]$$

so that the failure of Δ to be a derivation of the product is given by the bracket.

The definition of a BV algebra is then a Gerstenhaber algebra with such an operator, though alternative definitions exist in which Δ and the product are primary and the bracket is defined by the above equation. From the operadic/higher-homotopy point of view, one can then go on to consider BV_∞ algebras.

Recall that A_∞-algebras and L_∞-algebras (among others) can be characterized by an "inner" coderivation $d=[m,\ ]$ of square zero on an appropriate "standard" construction. In the context of BV algebras, where the bracket is more commonly written as {,}, the classical action is an element S_0 such that $\{S_0,S_0\}=0$ or, equivalently, $d=\{S_0,\ \}$ is of square zero. The quantum analog S is a perturbation of S_0 and satisfies instead

$$\{S,S\} = \Delta S \qquad [16]$$

This was originally called the "master equation," but now is increasingly referred to as a "Maurer–Cartan" equation.

Insertion Operads

There is another class of operads illustrated by trees (and more generally graphs) with a very different sort of "composition," namely insertion of one graph into another. The most directly relevant to physics is the kind of insertion used by Connes and Kreimer in their Hopf algebra constructed for renormalization of Feynman diagrams. For example, consider all finite graphs with exactly two external edges and internal numbered edges. Given two graphs Γ_1,Γ_2, define $\Gamma_1 \circ_i \Gamma_2$ by cutting edge i of Γ_1 and identifying the dangling edges with the two external edges of Γ_2.

For planar trees, yet another insertion operad is obtained by Chapoton, isolating a part of a structure due to Kontsevich, in which a small neighborhood of a vertex of the second planar tree is removed and the dangling edges are attached to a vertex of the first tree by entering through the angles between the edges at that vertex (**Figure** 7).

Inside the $\mathcal{HG}$-operad is the operad $\mathcal{B}race$ for an abstract brace algebra (forgetting the cup product), first described as such by Chapoton using the insertion operations of Kontsevich and Soibelman.

A_∞-Categories

Also of importance for applications to mathematical physics is the notion of an A_∞-category, first made explicit by Fukaya and now playing a major role in string D-brane theory and homological mirror symmetry. The D-branes are the objects of the A_∞-category and the open strings with boundaries on two (possibly equal) D-branes B_1,B_2 are the morphisms from B_1 to B_2. The operations m_i are defined only on tuples $(a_1,\ldots,a_i)$ of "composable" morphisms (e.g., strings).

PROPs

While an operad is an abstraction of a family of composable functions of n variables for various n, a PROP is an abstraction of a family of functions in

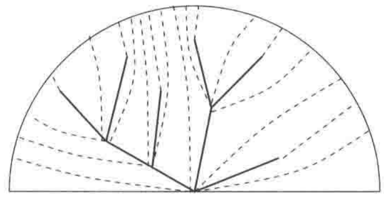


Figure 7 Angles determined by edges with leaves extended to the semicircle.

$\mathrm{Hom}(A^{\otimes p}, A^{\otimes q})$ for all p and q. Now the relevant images are graphs with p input legs and q output legs with composition being defined by grafting output legs of one graph to inputs of another. Feynman diagrams are the obvious example in physics or, in conformal field theory, tubular neighborhoods of such graphs, which is to say, Riemann surfaces with boundary circles: p as inputs and q as outputs.

See also: Algebraic Approach to Quantum Field Theory; Batalin–Vilkovisky Quantization; Constrained Systems; Deformations of the Poisson Bracket on a Symplectic Manifold; Deformation Quantization; Deformation Theory; Hopf Algebra Structure of Renormalizable Quantum Field Theory; String Field Theory.

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Operator Product Expansion in Quantum Field Theory

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Introduction

The operator product expansion (OPE) provides an algebraic structure in quantum field theory. In a sense it supercedes or rather transcends the equal-time commutation relations, which provide the traditional starting point for the canonical quantization of any quantum field theory. The essential idea is that for any two local operator quantum fields at spacetime points x_1, x_2 their product may be expressed in terms of a series of other local quantum fields at a point x, which may be identified with x_1 or x_2, times c-number coefficient functions which depend on $x_1 - x_2$. The set of operators which may appear depends on the particular quantum field theory and must of course be in accord with any requirements of conserved quantum numbers. The coefficient functions depend on $x_1 - x_2$ in a fashion which depends on the dimensions of the various operators involved, at least up to renormalization group corrections. The most singular contributions are those for the operators appearing in the OPE with lowest scale dimension. From a phenomenological point of view, only the first few terms in the OPE are of relevance. However, theoretically, especially for conformal field theories, it is desirable to know the full expansion to all orders in powers of $x_1 - x_2$ in such a way that the operator product may

be replaced by the full expansion in appropriate correlation functions. We first discuss the OPE for free theories and then the interacting case.

Free Field Theory

The OPE is most straightforward in free field theory when it almost reduces to a Taylor series expansion. For a simple free massless scalar field $\phi(x)$ then in four dimensions we may write

$$\phi(x)\phi(0) = \frac{C}{x^2} + :\phi(x)\phi(0): \quad [1]$$

where :: denotes normal ordering (moving all annihilation operators to the right of creation operators) and C is just a normalization numerical constant (for canonical normalization $C = 1/4\pi^2$). The $1/x^2$ term proportional to the identity operator reflects the leading singular behavior at short distances of $\phi(x)\phi(0)$, the power being determined by ϕ having dimension 1. For the normal-ordered term we may expand in terms of an infinite set of local operators by using the Taylor expansion

$$:\phi(x)\phi(0): = \sum_{n=0}^{\infty} \frac{1}{n!} x^{\mu_1} \cdots x^{\mu_n} :\partial_{\mu_1} \cdots \partial_{\mu_n} \phi(0)\phi(0): \quad [2]$$

where the operator appearing in the nth term has dimension $n+2$. Manifestly at short distances only the leading terms are relevant. Equation [1] also provides a point splitting definition of the local composite operator $:\phi^2(0):$ in terms of limit of $\phi(x)\phi(0)$ as $x \to 0$ after subtraction of the singular C/x^2 term.

The OPE can be easily generalized to composite operators defined by normal ordering. For $:\phi^2:$ we have, by applying Wick's theorem,

$$\begin{aligned} :\phi^2(x)::\phi^2(0): = {} & \frac{2C^2}{x^4} + \frac{4C}{x^2} :\phi(x)\phi(0): \\ & + :\phi^2(x)\phi^2(0): \end{aligned} \quad [3]$$

where Taylor series expansion may be applied to both $:\phi(x)\phi(0):$ and also $:\phi^2(x)\phi^2(0):$ to give an infinite sequence of local operators of increasing dimensions.

The expansion in terms of local operators may be reordered. For instance, from [1] we may write, using $\partial^2\phi = 0$,

$$\begin{aligned} \phi(x)\phi(0) = {} & \frac{C}{x^2} \\ & + \left(1 + \tfrac{1}{2}x^\mu\partial_\mu + \tfrac{1}{4}x^\mu x^\nu \partial_\mu\partial_\nu + \tfrac{1}{16}x^2\partial^2\right) :\phi^2(0): \\ & - \tfrac{1}{2}x^\mu x^\nu T_{\mu\nu} + O(x^3) \end{aligned} \quad [4]$$

where

$$T_{\mu\nu} = :\partial_\mu\phi\partial_\nu\phi: - \tfrac{1}{4}\eta_{\mu\nu} :\partial\phi \cdot \partial\phi: \quad [5]$$

is the energy–momentum tensor. In [4], and also in a similar context subsequently, we define $\partial :\phi^2(0): = \partial_y :\phi^2(y):|_{y=0}$. The expansion [4] provides a point splitting definition of $T_{\mu\nu}$ and also demonstrates that many operators appearing in the OPE are expressible in terms of overall derivatives of lower-dimension operators. We may also note that without further input there is an ambiguity in the definition of $T_{\mu\nu}$ of the form

$$T_{\mu\nu} \sim T_{\mu\nu} + a(\partial_\mu\partial_\nu - \tfrac{1}{4}\eta_{\mu\nu}\partial^2) :\phi^2: \quad [6]$$

In a conformal theory, however, we require $a = -1/6$.

Interacting Theories

The OPE becomes an essential tool in the context of interacting quantum field theories. For renormalizable quantum field theories various results can be proved to all orders in the standard perturbative expansion and are naturally assumed to be properties of the complete theory. In interacting theories we may no longer use normal ordering to define composite operators which, in general, have anomalous dimensions. The coefficient functions appearing in the OPE also gain perturbative corrections but these are constrained by renormalization group (RG) Callan–Symanzik equations.

Again if we consider the simplest case of a massless scalar theory as above but now with a renormalized coupling constant g the leading terms in the expansion of $\phi(x)\phi(0)$ are of the form (here we assume a Z_2 symmetry under $\phi \to -\phi$, otherwise the operator ϕ would be expected to appear in the OPE)

$$\phi(x)\phi(0) = \frac{C(g, \mu^2x^2)}{x^2} + D(g, \mu^2x^2)\phi^2(0) + \cdots \quad [7]$$

where μ is an arbitrary renormalization scale. This arbitrariness is reflected in the RG equation

$$\left(\mu\frac{\partial}{\partial\mu} + \beta(g)\frac{\partial}{\partial g} + 2\gamma_\phi(g)\right) C(g, \mu^2x^2) = 0 \quad [8]$$

At a fixed point $\beta(g_*) = 0$ this equation may be solved with an arbitrary choice of normalization to give $C(g_*, \mu^2x^2) = (\mu^2x^2)^{-\gamma_\phi(g_*)}$, which corresponds to the fields ϕ having a modified scale dimension $1 + \gamma_\phi(g_*)$. In a similar fashion the coefficient $D(g, \mu^2x^2)$ in [7] satisfies

$$\begin{aligned} & \left(\mu\frac{\partial}{\partial\mu} + \beta(g)\frac{\partial}{\partial g} + 2\gamma_\phi(g) - \gamma_{\phi^2}(g)\right) \\ & \quad \times D(g, \mu^2x^2) = 0 \end{aligned} \quad [9]$$

where it is necessary to introduce a new anomalous dimension function $\gamma_{\phi^2}(g)$ related to the composite

operator ϕ^2. Although it is natural to label the operator as ϕ^2 its definition in terms of the elementary field ϕ is essentially only as given in terms of the OPE [9]. At a fixed point again $D(g_*, \mu^2x^2) = k(\mu^2x^2)^{-\gamma_\phi(g_*)+(1/2)\gamma_{\phi^2}(g_*)}$, where the coefficient k is determined by the scale of the three-point function $\langle\phi(x)\phi(y)\phi^2(0)\rangle$. In asymptotically free theories the RG equations show that at short distances the coefficient functions tend to those of free field theory but with calculable logarithmic corrections. More generally, for a set of operators $\{O_i\}$ the OPE has the form

$$O_i(x)O_j(0) \sim \frac{1}{(x^2)^p}\sum_k C_{ijk}(g, \mu^2x^2)O_k(0) \qquad [10]$$

where p is determined by the free scale dimensions of the O_i and

$$\begin{aligned}&\left(\mu\frac{\partial}{\partial\mu} + \beta(g)\frac{\partial}{\partial g}\right)C_{ijk}(g, \mu^2x^2)\\ &\quad = \sum_n \big(\gamma_{kn}(g)C_{ijn}(g, \mu^2x^2) - \gamma_{in}(g)C_{njk}(g, \mu^2x^2)\\ &\qquad\qquad - \gamma_{jn}(g)C_{ink}(g, \mu^2x^2)\big)\end{aligned} \qquad [11]$$

with $\gamma_{in}(g)$ the anomalous dimension matrix arising from the mixing of composite operators.

An important aspect of the OPE is that the coefficient functions may be calculated perturbatively, essentially by applying the OPE in some suitable correlation function. Essentially the OPE provides a factorization between short-distance UV singularities and nonperturbative effects. In a Feynman graph the short distances in an operator product correspond to the large-momentum behavior and power-counting theorems allow a factorization up to calculable logarithmic corrections. A detailed analysis depends on the detailed technicalities of the proofs of renormalization to all orders of perturbation theory.

The coefficient functions in the OPE should be independent of any infrared or nonperturbative long-distance effects (such as confinement in QCD). However, the operators which appear in the OPE, such as ϕ^2 above, may have nonzero expectation values which are absent to all orders in perturbation theory.

Perturbative Example

The general considerations can be illustrated by considering a scalar field theory to lowest order in a perturbative expansion. We consider a four dimensional theory with a single scalar field and a potential $V(\phi) = \frac{1}{2}m^2\phi^2 + \frac{1}{24}g\phi^4$. Using dimensional regularization m^2, as well as g, is treated as a coupling with an associated β-function $\gamma_{\phi^2}(g)m^2$. With a mass term the operator ϕ^2 mixes with the identity operator so that

$$\begin{aligned}&(\mathcal{D} + \gamma_{\phi^2}(g))\langle\phi^2(0)\rangle = -\gamma_{\phi^2 I}(g)m^2\\ &\mathcal{D} = \mu\frac{\partial}{\partial\mu} + \beta(g)\frac{\partial}{\partial g} + \gamma_{\phi^2}(g)m^2\frac{\partial}{\partial m^2}\end{aligned} \qquad [12]$$

where $\gamma_{\phi^2 I}$ reflects the mixing. At one loop order we have

$$\beta(g) = \frac{3g^2}{16\pi^2}, \quad \gamma_{\phi^2}(g) = \frac{g}{16\pi^2}, \quad \gamma_{\phi^2 I}(g) = \frac{1}{8\pi^2} \qquad [13]$$

and we may also set $\gamma_\phi(g) = 0$. In this case in the operator product expansion (7) the coefficient C also depends on m^2x^2 and the RG equations [8] and [9] are now modified to include the effects of mixing

$$\begin{aligned}&\mathcal{D}C(g, m^2x^2, \mu^2x^2) = m^2x^2\gamma_{\phi^2 I}(g)D(g, \mu^2x^2)\\ &(\mathcal{D} - \gamma_{\phi^2}(g))D(g, \mu^2x^2) = 0\end{aligned} \qquad [14]$$

From lowest order perturbation theory with [13], and using [14] to include all orders in $g\ln\mu^2x^2$, we have in this approximation

$$\begin{aligned}&C(g, m^2x^2,\ \mu^2x^2)\\ &\quad = \frac{1}{4\pi^2} - \frac{2m^2x^2}{g}\left(1 + \frac{3g}{32\pi^2}\ln\mu^2x^2\right)^{2/3}\\ &\qquad \times\left(\left(1 + \frac{3g}{32\pi^2}\ln\mu^2x^2\right)^{-1/3} - 1\right)\\ &D(g, \mu^2x^2) = \left(1 + \frac{3g}{32\pi^2}\ln\mu^2x^2\right)^{1/3}\end{aligned} \qquad [15]$$

The operator product expansion then reproduces the small x behavior of the two point function $\langle\phi(x)\phi(0)\rangle$ at one loop, expanding C, D to first order in g, if we take

$$\langle\phi^2(0)\rangle = -\frac{m^2}{8\pi^2}\ln\frac{\mu}{m} + O(g) \qquad [16]$$

which is in accord with [12]. If $m^2 < 0$ the symmetry $\phi \leftrightarrow -\phi$ is broken and it is necessary to shift the field $\phi = \nu + f$, with $\nu^2 = -6m^2/g$ and the field f has a mass m_f with $m_f^2 = -2m^2$. The operator product expansion [7] with the same coefficient functions as in [15] remains valid. The two point function $\langle\phi(x)\phi(0)\rangle$, which includes a nonperturbative term ν^2, is again reproduced for small x at one loop now if

$$\langle\phi^2(0)\rangle = -\frac{6m^2}{g} - \frac{m^2}{2\pi^2}\ln\frac{\mu}{m_f} + O(g) \qquad [17]$$

but in this case it is necessary to expand $D(g, \mu^2x^2)$ to $O(g^2)$ as a consequence of the leading $1/g$ term in [17]. Note that both [16] and [17] contain the nonperturbative dependance on $\ln m$ and $\ln m_f$ which is present in the two point function.

Conformal Field Theories

When the β-function vanishes and a quantum field theory enjoys conformal invariance the operator product expansion is a potentially convergent expansion. It is natural to restrict to conformal quasiprimary operators which do not mix with lower scale dimensions under conformal transformations. If we consider, for instance, two scalar operators ϕ with scale dimension Δ_ϕ then the OPE has the generic form

$$\phi(x)\phi(0) = \frac{1}{x^{2\Delta_\phi}} + \sum_I C_{\phi\phi O^I} \frac{1}{(x^2)^{1/2}(2\Delta_\phi - \Delta^I + \ell)} \times C_{\Delta^I}^{(\ell)}(x,\partial)^{\mu_1,\ldots,\mu_\ell} O^I_{\mu_1,\ldots,\mu_\ell}(0) \quad [18]$$

where there is a sum over quasiprimary operators $O^I_{\mu_1,\ldots,\mu_\ell}$ with scale dimension Δ^I and spin ℓ, so they are symmetric traceless tensors of rank ℓ. In the first term in [18] the coefficient is chosen to be 1 by a choice of normalization. The coefficients $C_{\phi\phi O^I}$, with a standard normalization for O^I, are then determined by the coefficients of the corresponding three-point functions involving $\phi\phi$ and O^I. In [18] $C_{\Delta^I}^{(\ell)}$ are differential operators which sum up the contributions of all derivatives or descendants of the quasiprimary operator O^I. They can be explicitly given in terms of an integral representation, for any spacetime dimension, where the scale is fixed by requiring for the leading term $C_{\Delta^I}^{(\ell)}(x,0)^{\mu_1,\ldots,\mu_\ell} = x^{\mu_1}\cdots x^{\mu_\ell}$ – traces. The spectrum of operators which appear is obviously a property of the particular conformal field theory.

Ward Identities

If the theory has a symmetry with corresponding conserved currents then there are Ward identities which constrain the OPE of fields with the conserved current. For a current $J_{\mu a}$ then we have, in d dimensions, the singular contribution in the OPE is given by

$$J_{\mu a}(x)O(0) \sim -\frac{1}{S_d}\frac{x_\mu}{(x^2)^{(1/2)d}} t_a O(0) \quad [19]$$

where t_a are a set of matrix generators corresponding to the symmetry acting on the fields O and S_d is the volume of the unit $(d-1)$-dimensional sphere, $S_4 = 2\pi^2$. For a conserved current there are no anomalous dimensions and the coefficient in [19], which depends on the normalization for the current $J_{\mu a}$, is chosen so that $[Q_a, O(0)] = -t_a O(0)$ with Q_a the charge formed from $J_{\mu a}$. For the energy–momentum tensor the operator there is an analogous result. We consider the simpler case of a conformal theory when the energy–momentum tensor is both conserved and traceless and

$$T_{\mu\nu}(x)O(0) \sim A_{\mu\nu}(x)O(0) + B_{\mu\nu\lambda}(x)\partial^\lambda O(0) + \cdots \quad [20]$$

where $A_{\mu\nu}(x) = O(x^{-d})$ and $B_{\mu\nu\lambda}(x) = O(x^{-d+1})$. As a distribution $A_{\mu\nu}(x)$ is ambiguous up to terms proportional to $\delta^d(x)$. If Δ is the scale dimension of O and $s_{\mu\nu}$ are the Lorentz spin generators acting on O the Ward identities then give

$$\partial^\mu A_{\mu\nu}(x) = \left(\frac{\Delta}{d}\eta_{\nu\lambda} + C_{\nu\lambda} + \tfrac{1}{2}s_{\nu\lambda}\right)\partial^\lambda\delta^d(x)$$

$$\begin{aligned} A_{\mu\mu}(x) &= C_{\mu\mu}\delta^d(x) \\ \partial^\mu B_{\mu\nu\lambda}(x) &= -\eta_{\nu\lambda}\delta^d(x) \end{aligned} \quad [21]$$

where $C_{\mu\nu}$ is a constant tensor reflecting the arbitrariness in $A_{\mu\nu}$, it is immaterial as far as Ward identities are concerned. We may choose

$$\frac{\Delta}{d}\eta_{\nu\lambda} + C_{\nu\lambda} = 0 \quad [22]$$

(If desired, we might also take $A'_{\mu\nu}(x) = A_{\mu\nu}(x) + (1/2)s_{\mu\nu}\delta^d(x)$ in which case $\partial_\mu A'_{\mu\nu}(x) = 0$, $A'_{[\mu\nu]}(x) = (1/2)s_{\mu\nu}\delta^d(x)$ but such an antisymmetric piece seems unnatural). In general there is no unique form for $A_{\mu\nu}(x)$, as a consequence of the freedom of choice for $C_{\nu\lambda}$ in [21]. However, for a scalar field O we must have, for $x \neq 0$,

$$\begin{aligned} A_{\mu\nu}(x) &= \frac{\Delta}{d-1}\frac{1}{S_d}\left(\eta_{\mu\nu} - d\frac{x_\mu x_\nu}{x^2}\right)\frac{1}{(x^2)^{(1/2)d}} \\ &= -\frac{\Delta}{(d-1)(d-2)}\frac{1}{S_d}\partial_\mu\partial_\nu\frac{1}{(x^2)^{(1/2)d-1}} \end{aligned} \quad [23]$$

with the overall scale determined by [21].

For the operator product of the current $J_{\mu a}$ with itself there is an additional term proportional to the identity operator of the form

$$J_{\mu a}(x)J_{\nu b}(0) \sim C_J\delta_{ab}\left(\eta_{\mu\nu} - 2\frac{x_\mu x_\nu}{x^2}\right)\frac{1}{x^{2(d-1)}} \quad [24]$$

where the coefficient C_J, which determines the scale of the two-point function for $J_{\mu a}$, is well defined since the normalization of the current is determined through the Ward identity. A similar result also holds for the operator product of the energy–momentum tensor with itself, with an overall coefficient C_T. In general, we may also write for the operator product of two scalar fields O:

$$O(x)O(0) \sim C_O\frac{1}{x^{2\Delta}} - \frac{C_O}{C_T S_d}\frac{d\Delta}{d-1}\frac{1}{(x^2)^{\Delta-(1/2)d+1}} \times x^\mu x^\nu T_{\mu\nu}(0) \quad [25]$$

neglecting other contributions. The contribution of the energy–momentum tensor does not therefore introduce any new coefficient.

Two Dimensions

In two dimensions the OPE plays an essential role in the discussion of conformal field theories. For a Euclidean metric it is natural to use complex variables z and $\bar{z}$. The energy–momentum tensor in this case reduces to a chiral field $T(z)$ and its conjugate $\bar{T}(\bar{z})$. For the operator product with a chiral field $\phi(z)$ with scale dimension Δ,

$$T(z)\phi(0) \sim \frac{\Delta}{z^2}\phi(0) + \frac{1}{z}\phi'(0) \qquad [26]$$

and, for the operator product of T with itself,

$$T(z)T(0) \sim \frac{c}{2z^4} + \frac{2}{z^2}T(0) + \frac{1}{z}T'(0) \qquad [27]$$

Here c is the Virasoro central charge, which plays a critical role in the discussion of two-dimensional conformal field theories, it is given by the two-point function which follows from [27], $\langle T(z)T(0)\rangle = (1/2)cz^{-4}$.

In simple rational conformal field theories the operators are organized into conformal blocks by the infinite-dimensional extended conformal symmetry in two dimensions. This allows the full spectrum of operators and their dimensions to be determined and in consequence complete results for the OPE to be found in many cases.

Further Remarks

The OPE reflects the locality properties of quantum field theories and can be extended without difficulty to curved space backgrounds. For a product $\phi(x)\phi(0)$, the separation x^2 may be replaced by a biscalar at x and 0 but it is necessary to include in the OPE contributions involving the background Riemann tensor as well as the operator fields present in flat space. There is also a generalization of the OPE for superfields on superspace.

At a fundamental level although the OPE can be derived to all orders in perturbation theory the contribution of nonperturbative effects such as instantons to the coefficients is not entirely clear. Issues of associativity have yet to be fully analyzed.

There are also important applications to the phemenonological analysis of QCD when assumptions about the OPE and saturation of sum rules can lead to results for the vacuum expectation value of gauge-invariant operators such as $F^{\mu\nu}F_{\mu\nu}$.

See also: Boundary Conformal Field Theory; Effective Field Theories; Quantum Chromodynamics; Renormalization: General Theory; Renormalization: Statistical Mechanics and Condensed Matter; Two-Dimensional Models.

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Optical Caustics

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Introduction

Optical caustics are the bright forms created by the focalization, natural or artificial, of light (**Figure 1**). Special caustic points, called focuses, are produced by stigmatic optical systems in order to visualize objects. However, there are no special conditions for producing usual caustics. Every congruence of rays always generates a caustic, more or less intricate.

Caustics have been observed and described since a long time, tracing back to antiquity. The name itself was coined after the Greek root "kausticos" meaning burning and expressing that a high energy density is produced by ray focalization at a caustic point. Conceptually, they appeared in the literature as "evolutes," "envelopes," "centers of curvature," "focals," etc. However, these different approaches, often too restricted, were unable to clarify the

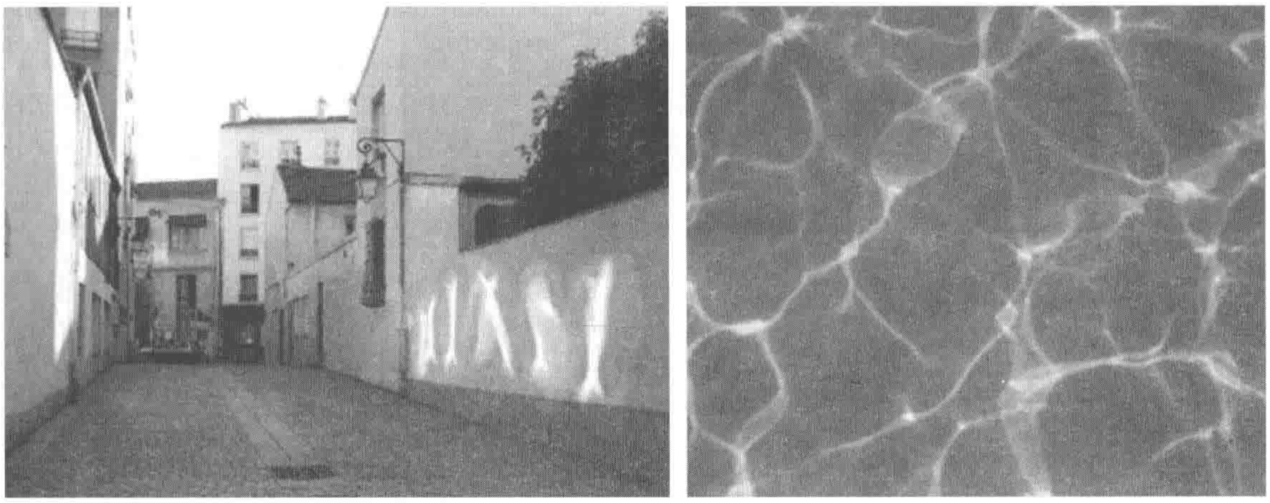


Figure 1 Optical caustics may be produced by reflection (on window glasses) or by refraction (through the wavy surface of a swimming pool). Here the light source, the Sun, has some angular extension and the caustic appears somewhat blurred.

general properties of caustics, for instance, their classification in generic types. This difficult question was solved only recently in the framework of the singularity theory which appeared in the second half of the twentieth century (Whitney 1955, Thom 1956). Caustics are now understood as physical realizations of Lagrangian singularities, and they are often called optical singularities or optical catastrophes.

The aim of this introductory article is to show in which sense caustics can be understood as singularities, and to present their main properties.

The Physical Phenomenon

Caustics are usually observed by interposing a screen on the ray trajectories and their trace in the screen forms a set of bright curves called "fold" (A_2). Across the fold, the number of rays passing through a given point jumps by ± 2. Two fold curves may join at some point forming there a tip called cusp (A_3). A simple example is provided by the nephroid that one sees in a cup of coffee when the light is reflected off the cylindrical sides. In the three-dimensional (3D) space, the folds form surfaces and the cusps form curves (**Figure 2**). For particular positions of the screen, three other types of caustics may be observed: the swallowtail (A_4), the meeting point of two cusp lines; the elliptic umbilic (D_4^-), the meeting point of three cusp lines; and the hyperbolic umbilic (D_4^+) where a cusp line tangentially meets a fold surface (**Figure 2**). These five caustic types are generic in the sense that any other type of caustic point is unstable and decomposes into these generic caustic points under small perturbations. The perfect focus is an example of a nongeneric caustic point, obtained by imposing a special symmetry. The natural focusing of light, as in gravitational optics, produces only generic caustics. A caustic point is then a generalized focus. The caustic surface is a complex surface in the 3D physical space, generally self-intersecting and possessing singular lines A_3 ending at singular points A_4, D_4^-, or D_4^+.

At the scale of the wavelength of the light, the caustics have a more complex structure. Instead of well-defined surfaces, lines and points, one observes a system of interference fringes concentrated in the vicinity of the geometrical caustic. Each type of caustic point has its own diffraction pattern (also called diffraction catastrophe) (**Figure 3**). These interference systems are easily produced, for instance, by focusing a coherent laser beam by a

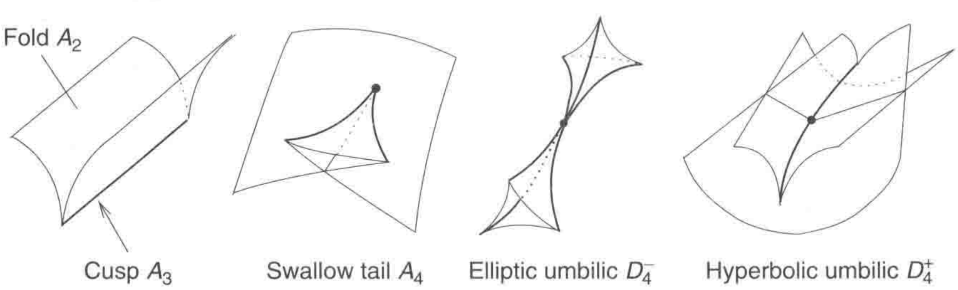


Figure 2 The five generic types of caustics of the 3D space.

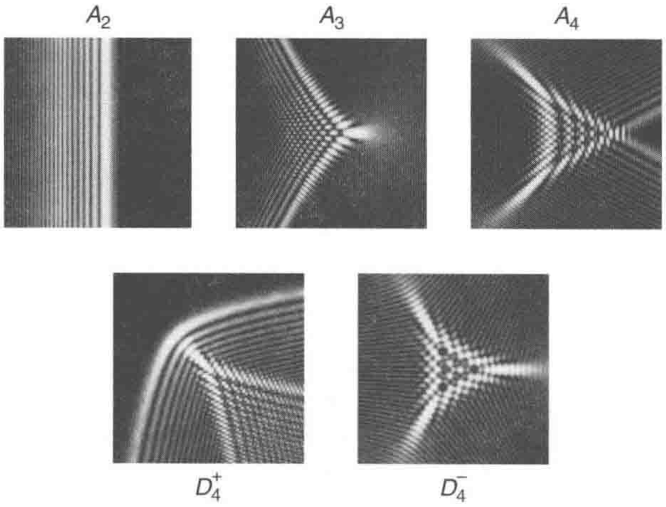


Figure 3 Interference fringes produced by the five generic caustics of the 3D space (numerical simulation).

corrugated glass or by a water droplet. An important feature is revealed by Gouy's experiment, in which bright and dark fringes are inverted when the rays are forced to pass through a focus (Guillemin and Sternberg 1977). The experiment shows that the wave undergoes a phase shift of $\pi/2$ when the associated ray passes through a caustic point.

So, caustics are fundamental objects of both the geometrical optics and the wave optics.

Modeling Caustics

Because of the presence of a caustic, a congruence of rays generally presents intersecting rays. At the points of intersection, the coordinates q_1, q_2, q_3 of the physical space R^3 are unable to distinguish the various intersecting rays and they do not constitute a convenient system of coordinates. It is then interesting to construct an abstract space in which the rays are represented by nonintersecting curves. The initial congruence is recovered by projecting the abstract space into the physical one. All the models use this type of construction in which the properties of the caustics are deduced from those of the projection.

Caustics as Envelopes of Rays

In this geometrical modeling, each ray is labeled by two parameters r_1, r_2, for instance, the coordinates on the initial wave front W. A third coordinate r_3 specifies the points along the ray, for instance, by assigning their distance to W. Taken together, these three coordinates represent the congruence of rays, and define a 3D space, the source space $M = \{r_1, r_2, r_3\}$. By construction, the rays in M do not intersect. The coordinates (q_1, q_2, q_3) of the current point $P \in R^3$ along each ray depend differentiably on the coordinates (r_1, r_2, r_3) and define a "projection" $f : (r_1, r_2, r_3) \mapsto (q_1, q_2, q_3)$ from the source space M into the physical space R^3.

The caustic points correspond to the envelope of the rays. At a caustic point P, the energy density flowing along the rays becomes infinite, since the small volume delimited by neighboring rays is shrunk into a small surface at P. This behavior may be simply expressed with the help of the projection f: the rank rk of the derivative Df is equal to 2 at the point representing P in M. This motivates the following definition. Given a map $f : M \to N$, a point $x \in M$ is said to be critical (or singular) if the rank of the derivative Df is less than the maximal possible value min(dim M, dim N). Here, $\dim M = \dim N = 3$, and a critical point is a point where rk < 3. The set $\Sigma \subset M$ of the critical points is called the singular set. The caustic C is the image of the singular set: $C = f(\Sigma)$. One also says that the caustic points are the critical values of f.

In practice, the derivative Df is expressed by the Jacobian matrix $J = \partial(q_1, q_2, q_3)/\partial(r_1, r_2, r_3)$ and the singular set Σ is defined by solving the equation

$$\det(J) = 0 \qquad [1]$$

If this equation permits one to express explicitly one coordinate, say r_3, as a function of the other two, the caustic surface C is found in parametric form: $q_1 = q_1(r_1, r_2, r_3(r_1, r_2))$, etc. For a homogeneous medium, equation [1] is of second degree in r_3 and the caustic is composed of two sheets which meet at the umbilic points D_4.

Equation [1] gives all caustic points independently of their nature, that is, it does not distinguish between A_2, A_3, A_4, D_4^-, and D_4^+. A refinement allows one to recognize different types of caustic points. One defines the Thom–Boardman class Σ^i as the points in M where Df has a kernel of dimension i. Then one defines inductively the class $\Sigma^{i,\dots,j,k}$ as the class Σ^k of the restriction of f to $\Sigma^{i,\dots,j}$. Thus, Σ^0 represents the regular points (noncaustic points), $\Sigma^{1,0}$ the fold points A_2, $\Sigma^{1,1,0}$ the cusp points A_3, $\Sigma^{1,1,1,0}$ the swallow-tail points A_4, and $\Sigma^{2,0}$ the umbilics D_4 (hyperbolic or elliptic). Altogether, the classes Σ^I, $I \neq 0$, form the singular set Σ.

The Thom–Boardman classes constitute a simple and powerful tool for computing the structure of a caustic. Each class is obtained by canceling some functional determinants associated with the map f or with its restriction to some class. However, the method presents the weakness of ignoring the special nature of a set of rays: its Lagrangian character. As a consequence, it is unable, for instance, to distinguish between D_4^- and D_4^+.

Caustics as Lagrangian Singularities

As for mechanics, the natural framework for geometrical optics is a phase space: the cotangent space $T^*R^3 = \{p_i, q_i\}$ of the configuration space $R^3 = \{q_i\}$. The phase space is characterized by its symplectic structure, that is, the differential 2-form $\omega = \sum_i \mathrm{d}p_i \wedge \mathrm{d}q_i$, which is nondegenerate and closed ($\mathrm{d}\omega = 0$).

A set of rays in the phase space is defined by specifying the wave vector (or momentum) $\boldsymbol{p}$ at each point $\boldsymbol{q}$ of the congruence. In the simple case where only one ray passes through each point, one has $\boldsymbol{p} = \nabla S$, where S is the optical length $\int n\,\mathrm{d}s$ and n the refractive index. In other words, $\boldsymbol{p}$ is the differential of the optical length. The wave vector $\boldsymbol{p}$ is tangent to the ray and orthogonal to the (geometrical) wave front $S = \text{const}$. The eikonal equation shows that its modulus is n. As a direct consequence of the relation $\boldsymbol{p} = \nabla S$, the symplectic form annihilates identically for these $\boldsymbol{p}$. However, in general, because of the presence of the caustics, one must not expect to have $\boldsymbol{p} = \nabla S$ for some function S. Nevertheless, it is possible to keep the more general property to annihilate ω. This motivates the definition of a Lagrangian submanifold: a submanifold $L \subset T^*R^3$ of dimension 3 (that is, half of the dimension of the phase space) on which the symplectic form vanishes: $\omega|_L = 0$. Every congruence of rays is described by a Lagrangian submanifold. The Lagrangian submanifold plays the same role as the source space in the preceding section. The role of the projection f is played by the natural projection π from the phase space into the configuration space $\pi(\boldsymbol{p}, \boldsymbol{q}) = \boldsymbol{q}$, or more precisely to its restriction to L: $f = \pi|_L$. It is called a Lagrangian map (or Lagrangian projection) and it is again a map between two spaces of the same dimension (here 3). When L is given by an embedding $\iota: L \to T^*R^3$, one has $f = \pi \circ \iota$. A caustic is then defined as the set of critical values of a Lagrangian map.

There exist two remarkable results showing that a Lagrangian submanifold may be described in terms of functions or of families of functions. As a consequence, caustics are not directly related to the singularities of maps but, more particularly, to the singularities of functions.

Generating function of a Lagrangian submanifold The 3D Lagrangian submanifold $L \subset \{p_i, q_i\}$ is locally defined by three coordinates $p_\alpha (\alpha \in A)$ and $q_\beta (\beta \in B)$ depending on the three other ones p_β and q_α: $p_\alpha = p_\alpha(q_\alpha, p_\beta)$, $q_\beta = q_\beta(q_\alpha, p_\beta)$. One can show that this may be done in such a way that each conjugate pair (q_i, p_i) gives exactly one independent variable and one dependent variable. Formally: $A \cup B = \{1, 2, 3\}$, $A \cap B = \emptyset$.

In fact, introducing the function $S(q_\alpha, p_\beta) = \int \langle p, \mathrm{d}q \rangle - \langle q_\beta, p_\beta \rangle$ ($\langle , \rangle$ denotes the scalar product), the local equation for L takes a more simple form:

$$q_\beta = -\frac{\partial S}{\partial p_\beta}, \qquad p_\alpha = \frac{\partial S}{\partial q_\alpha} \qquad [2]$$

The function S is well defined, since, by the definition of a Lagrangian submanifold $\int \langle p, \mathrm{d}q \rangle$ is locally path independent: it depends only on its end points. S is called a (local) generating function.

Formula [2] generalizes $\boldsymbol{p} = \nabla S$, to which it reduces when $B = \emptyset$, that is, for nonintersecting rays.

Generating family and optical catastrophes Formula [2] may be rewritten in an interesting way. Taking the $|B|$ variables p_β as internal parameters x and $q = (q_\alpha, q_\beta)$ as external parameters, we construct a function F of x parametrized by q: $F(x, q) = S(q_\alpha, x) + \langle q_\beta, x \rangle$. Now the Lagrangian submanifold L is defined by

$$L = \left\{ (q, p) \colon \exists x \colon \frac{\partial F}{\partial x} = 0,\ p = \frac{\partial F}{\partial q} \right\}$$

F is called the generating family. The first equation $\partial F / \partial x = 0$ determines the rays passing through the fixed external parameter $\boldsymbol{q} \in R^3$. The second one distinguishes these rays according to their wave vector $\boldsymbol{p}$. Each ray corresponds to a critical point (i.e., an extremum) of F considered as a function of x. At a caustic point, two infinitely close rays are converging and F then presents a degenerate critical point. So the generating-family technique links the caustics to the theory of singularities of functions depending on some parameters, that is, to the catastrophe theory (Thom 1969). Caustics are also called optical catastrophes.

The generating families are not uniquely defined, even locally. In optics, one may always take for F the equivalent family "optical length" d, considered as a function defined on the initial wave front W (this is discussed in the following).

Caustics as the Locus of Wave Front Singularities

There exists a remarkable duality linking rays and wave fronts. As a consequence, the caustic points (i.e., Lagrangian singularities) are related to singularities of wave fronts (i.e., Legendrian singularities). A typical wave front W may possess only two types of singularities: cuspidal curves and swallow-tail points. During the motion of W, governed by the eikonal equation, the cuspidal curves generate surfaces, and swallow tails generate curves. These surfaces are

exactly the fold surfaces of the caustic C and the curves are the cusp lines of C. The point singularities of the caustic, that is, the swallow tails and the umbilics, correspond to bifurcations of the instantaneous wave front, at certain moments of its motion.

Caustics as Short Wave Asymptotic

The fine observation of the optical caustics shows that they never appear as the well-defined surfaces given by the geometrical optics, but rather as diffraction patterns concentrated around these surfaces. So wave optics is the natural framework to account for this fundamental feature. One exploits the fact that the wave number $k = 2\pi/\lambda$ (λ: wavelength of the light) is a large parameter. This short-wave approximation permits the use of powerful expansion techniques and clarifies the relation with the geometrical optics viewpoint, formally obtained for k tending to infinity.

The stationary phase In the most simple model, the Huygens–Fresnel principle, the amplitude $U(P)$ of the optical field may be evaluated by adding the secondary disturbances emitted from the points Q of some initial wave front W:

$$U(P) = c \iint_W \frac{e^{ikd}}{d} G \, ds \qquad [3]$$

where d is the distance QP. G is the inclination factor, a smooth function defined on W and c some prefactor. For simplicity, G and n (the refractive index) are assumed to be constant. Defining $a = cG/d$, formula [3] appears as an integral of the form $\int a(y)e^{ik\phi(y)}dy$. This type of integral may be evaluated for large k by the method of stationary phase. The principal contributions are due to points where the phase ϕ is stationary: $\nabla\phi = 0$. For wave optics, ϕ is the length PQ, considered as a function of Q and parametrized by P. The stationary condition means that PQ is normal to W, that is, it represents a ray of geometrical optics. The function PQ is a generating family in the sense of the discussion earlier.

If no stationary points exist, that is, if P is in the shadow, the integral is $O(k^{-N})$ for any N. Otherwise, and if the critical points are not degenerate, the phase stationary method gives (Guillemin and Sternberg 1977):

$$U(P) = \frac{2\pi}{k} \sum_{\text{rays } PQ} e^{(1-\sharp)\pi i/2} \times \frac{a(Q)e^{ikd}}{|(1-\mu_1 d)(1-\mu_2 d)|^{1/2}} + O(k^{-2}) \qquad [4]$$

where μ_1^{-1} and μ_2^{-1} are the two principal radii of curvature at $Q \in W$, and $\sharp$ the number of caustic points (also called focal points) along the ray PQ.

In the stationary-phase approach, the caustic C, locus of centers of curvature of W, appears as an obstacle in constructing asymptotics, since formula [4] diverges when $d\mu_i \to 1$, that is, when P tends to C. It is, nevertheless, remarkable that C also appears explicitly when [4] is valid, via the μ_i's and $\sharp$. In particular, the term $e^{-\sharp i\pi/2}$, applied in the case of a focus ($\sharp = 2$), accounts for the phase shift of π observed in Gouy's experiment.

Asymptotics on caustics Uniform asymptotic formulas, valid also on the caustic, need a more complex theoretical framework, for instance, Maslov's theory, presented here in a necessarily simplified version (see Maslov and Fedoriuk (1981) for more detail).

The starting point is the equation of wave optics, that is, the Helmholtz equation

$$(\Delta + k^2 n^2)U = 0 \qquad [5]$$

where the refractive index n generally varies from point to point. For $k \to \infty$, one looks for an asymptotic solution in the (tentatively) form:

$$U(P) = e^{ikS(q_1,q_2,q_3)} \sum_{j=0}^{\infty} (ik)^{-j} \varphi_j(q_1, q_2, q_3) \qquad [6]$$

Inserting this form in eqn [5] one obtains the eikonal equation (or characteristic equation) for the phase S:

$$(\nabla S)^2 = n^2$$

and an infinite series of equations for the amplitudes φ_j, called the transport equations. One knows that the Cauchy problem for the eikonal equation may be reduced to the integration of the corresponding Cauchy problem for the Hamilton system (or bicharacteristic system):

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = 2p, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q} = \nabla n^2$$

where $H = \langle p, p \rangle - n^2$. Its solutions, the bicharacteristics $q(t, \xi)$, $p(t, \xi)$ are parametrized by the "time" t and the 2D parameter ξ parametrizing the points on the initial wave front W. The bicharacteristics form a 3D Lagrangian submanifold L in the phase space $\{p_i, q_i\}$ and one recovers the preceding situation. Assuming L to be simply connected, one defines a global phase function S on L by formula $S(t, \xi) = \int \langle p, dq \rangle$.

In a domain $\Omega_j \subset L$ not containing the singular set and in which the coordinates t, ξ are in a one-to-one correspondence with the physical coordinates, S

becomes a function of q_i. Using the transport equation, one finds the leading term of the asymptotic solution (with accuracy to k^{-1}) in the following form:

$$U(P) = (K(\Omega_j)\varphi)(q) = \sqrt{\left|\frac{d\sigma}{dq_i}\right|}e^{ikS(q_1,q_2,q_3)}\varphi(q_1,q_2,q_3) \quad [7]$$

where $d\sigma$ and dq_i, respectively, represent the measures on the Lagrangian submanifold and on the physical space. The amplitude φ depends on the initial conditions. Formula [7] defines a precanonical operator $K(\Omega_j)$. It has the same form as [4], with the same drawback to diverge near the singular set Σ, where $dq_i = 0$.

In a domain Ω_j containing the singular set, L is locally parametrized by mixed coordinates q_α, p_β. The basic idea is then, roughly speaking, to carry out a Fourier transform F_k with respect to these p_β (in fact, a variant of the usual Fourier transform, in which the parameter k appears in the prefactor and in the phase term). This leads one to consider, instead of $\mathcal{L} = \Delta + k^2n^2$, the operator $\hat{\mathcal{L}} = F_k\mathcal{L}F_k^{-1}$, and instead of U, the unknown function $V = F_kU$. In this Fourier space, V may be found in the same way as U was found in the preceding case, with S replaced here by the local generating function $S_j(q_\alpha, p_\beta) = S - \langle q_\beta, p_\beta\rangle$. Coming back to the real space by F_k^{-1}, one obtains (with the same accuracy):

$$U(P) = (K(\Omega_j)\varphi)(q) = F_k^{-1}\left[\sqrt{\left|\frac{d\sigma}{dp_\beta dq_\alpha}\right|}e^{ikS_j(q_\alpha,p_\beta)}\varphi(q_\alpha,p_\beta)\right] \quad [8]$$

There is no divergence in this local solution. So local short-wave asymptotics may be found everywhere, even on the caustic where they have a more complex form than the form [6] or [7].

Global asymptotics and Maslov's index The global asymptotic solution is obtained by formally gluing the local solutions by a partition of unity $\Sigma e_j = 1$ subordinate to a covering $\{\Omega_j\}$ of L. However there is a difficulty. The representations of the same precanonical operator in different local coordinates q_α, p_β, even not containing the singular set, agree only up to a constant multiplier $e^{i\pi m/2}$, where the integer m is the number of negative eigenvalues of some matrix. One is led to multiply every precanonical operator by a convenient phase factor $e^{-i\pi\gamma/2}$, where $\gamma \in Z_4$ is called Maslov's index. The coherency of the phase factor in different domains is realized by using the important property of Σ to be co-oriented. Thus, γ counts the number of passages of an oriented path on L from the negative side of Σ to its positive side, minus the number of passages in the opposite sense. Maslov's index is locally constant and jumps by ± 1 only across the singular set Σ. The global canonical operator is now formally defined as $K = \Sigma_j e^{-i\pi\gamma_j/2}K(\Omega_j)e_j$.

Finally, the canonical operator K is well defined only if it is independent of the $\{\Omega_j\}$ and e_j used for its definition. This possibility is expressed (in the case of a simply connected L) by the following property, intrinsically attached to L: the Maslov index cancels on every closed loop. So the only obstruction for global asymptotics is the nontriviality of the characteristic class defined by Maslov's index and not the caustic.

The central object of the caustic modeling is then the projection of the submanifold representing the rays (M or L) into the physical space. The possibility to reduce this projection to some normal form is the key result for the local classification of caustics.

Local Classification of Caustics

Equivalence, Stability, and Genericity

In order to distinguish different types of singularities, one has to define an equivalence relation. Two Lagrangian maps $f_i : T^*M_i \supset L_i \to M_i$ $(i = 1, 2)$, are said to be Lagrange equivalent if there is a diffeomorphism $h : T^*M_1 \to T^*M_2$ preserving both the symplectic and the fiber structures, and sending L_1 to L_2. In fact, only the local problem of classification makes sense, and one considers, instead of Lagrangian maps, germs of Lagrangian maps. A map germ is a map locally defined, that is, defined in an infinitely small neighborhood around a point (depending on the germ). The notion of Lagrange equivalence is extended to the germs. A Lagrangian singularity is then the Lagrange equivalence class of a germ at a critical point. Each equivalence class represents a type of Lagrangian singularity, that is, a type of caustic point.

The example of the perfect focus point shows that there exist singularities which are totally unstable. In this sense, they correspond to idealized situations not physically realizable, and they have to be disregarded. Conversely, stable singularities resist under the action of small perturbations. They correspond to Lagrangian germs for which all neighboring germs are Lagrange equivalent (not necessarily at the same point, but near the point considered).

Now the important question is: do the stable germs represent the generality? In the best case, stable germs form a dense open set. This means that every germ may be approximated by stable germs. In this case, one says that the stable germs are generic.

Stability and genericity are disctinct notions. It turns out that they coincide for low values of the dimension n of the "physical space" ($n < 6$), but they may disagree at higher dimensions.

Classification of Stable Caustics

The fundamental result of the theory is the local classification of Lagrangian singularities (Arnol'd 1972). With the help of the generating families, the study of Lagrangian singularities is reduced to the study of singularities of families of functions. More precisely, at a singular point, every stable Lagragian map is equivalent to one of the following maps, given by their generating function S and by their generating family F:

$$
\begin{aligned}
A_2: \quad & S = p_1^3 \\
& F = x^3 + q_1 x \\
A_3: \quad & S = \pm p_1^4 + q_2 p_1^2 \\
& F = \pm x^4 + q_1 x^2 + q_2 x \\
A_4: \quad & S = p_1^5 + q_2 p_1^3 + q_3 p_1^2 \\
& F = x^5 + q_1 x^3 + q_2 x^2 + q_3 x \\
D_4^{\pm}: \quad & S = p_1^3 \pm p_1 p_2^2 + q_3 p_1^2 \\
& F = x_1^2 x_2 \pm x_2^3 + q_1 x_2^2 + q_2 x_2 + q_3 x_1
\end{aligned}
$$

These polynomial functions are called normal forms. The stable singularities are generic. In other words, every other type of singularity is destroyed by infinitely small perturbations and gives a set of singularities belonging to the list. The five generic caustics have been observed and experimentally studied in detail (Berry and Upstill 1980, Nye 1999).

By inserting the normal forms S in a short-wave asymptotic, one obtains the diffraction patterns associated with the five caustic types (**Figure 3**). They generalize the Airy function which corresponds to the fold singularity.

The normal forms describe at once the geometry of the caustics and the interference systems around them.

Codimension, Corank, Multiplicity, and Index

Lagrangian singularities are also characterized by some numbers. They have a codimension c equal to the difference between the dimension of the physical space and their dimension: $c(A_2) = 1$, $c(A_3) = 2$, $c(A_4) = c(D_4^{\pm}) = 3$. They have a corank ck, equal to the difference between the dimension of the space and the rank of the Lagrangian map: $\mathrm{ck}(A_2) = \mathrm{ck}(A_3) = \mathrm{ck}(A_4) = 1$, $\mathrm{ck}(D_4^{\pm}) = 2$. The corank is the number of internal parameters of the generating family F. They also have a multiplicity μ, which is the number of nondegenerate critical points of F, that is, the number of rays coinciding at the singularity. In the 3D space, one has $\mu = c + 1$: $\mu(A_2) = 2$, $\mu(A_3) = 3$, $\mu(A_4) = \mu(D_4^{\pm}) = 4$.

Short-wave asymptotics near the caustic present remarkable scaling properties (Berry and Upstill 1980). In particular, the amplitude $|U(P)|$ increases like k^{δ} as $k \to \infty$. The number δ depends only on the type of the singularity and it is called the singularity index. The more "degenerate" the singularities, the larger the index, and then the brighter the caustic point: $\delta(A_2) = 1/6 < \delta(A_3) = 1/4 < \delta(A_4) = 3/10 < \delta(D_4^{\pm}) = 1/3$.

Global Organization of Caustics

The global properties of caustics are less understood than the local ones. There is, nevertheless, an interesting result concerning specifically the caustics in the 3D space (Chekanov 1986). Given a Lagrangian map $f: L \to R^3$, the Euler characteristic $\chi(\Sigma)$ of the singular set $\Sigma \subset L$ and the number $\sharp D_4(-1/2)$ of umbilics of index –1/2 are related by the formula

$$\chi(\Sigma) + 2\sharp D_4(-1/2) = 0 \qquad [9]$$

At an umbilic point T, Σ is locally a cone with vertex at T. The index is defined according to the relative positions of the following elements: the 2D plane $\Pi = \ker f$, the cusp lines $A_3 \subset \Sigma$ passing through T, and the characteristic line l which represents the ray at T. If l and A_3 are separated by Π, the index is equal to $+1/2$, and to $-1/2$ in the other case. The index of an elliptic umbilic is always equal to $-1/2$.

The validity of Chekanov's formula [9] requires that L lies on a hypersurface E of the phase space, convex with respect to the wave vectors. The characteristics are the orthocomplements of E. In this framework, the singularities are called optical singularities, because such an E is always defined in geometrical optics by the eikonal equation. All Lagrangian singularities can be realized as optical singularities. Chekanov's formula has been experimentally checked (Joets and Ribotta 1996).

The Chekanov relation has an important consequence on the caustic bifurcations (also called metamorphoses or perestroikas), that is, the generic transformations modifying the topology of a caustic depending on one parameter. Among the 11 possible caustic bifurcations, considered as bifurcations of general Lagrangian singularities, four of them cannot be realized as bifurcations of optical Lagrangian singularities. So Chekanov's relation reduces the number of optical metamorphoses to seven.

Extensions

Caustics in Spaces of Higher Dimension

The local classification of Lagrangian singularities has been extended in spaces of higher dimension. For $n=4$, in addition to the preceding ones, two new singularities appear: the butterfly A_5 and the parabolic umbilic D_5. For $n=5$, in addition to A_6 and $D_6^{\pm}$, one has a new type of umbilic: E_6. However, in higher dimensions, the classification becomes more complex. In addition to stable singularities, like those of the series A_i, D_i, E_i, one encounters unstable generic singularities which depend on arbitrary parameters (moduli). Despite this difficulty, there exists a classification of generic Lagrangian singularities up to the dimension $n=10$.

The Maslov index has been extended in spaces of higher dimension and has led to the discovery of invariants associated with particular types of singularities (Vassilyev 1988). These invariants control the number of some types of singularities. For instance, in dimension $n=4$, the number of A_5 (taking account of sign) is equal to zero.

Symmetrical Caustics

Another extension consists in imposing some constraint, for instance, a symmetry (Janeczko and Roberts 1993). Symmetrical caustics are not merely the symmetrized usual caustics. Many of them result from the stabilization of unstable singularities of higher codimension by the symmetry. For example, in the 3D space, the butterfly A_5 is unstable, but the symmetrical butterfly is a generic singularity in the class of Lagrangian singularities having the mirror symmetry.

Nonoptical Caustics

Caustics, as locus of focalization, are not restricted to the usual optics. They are also observed in electronic optics or in gravitational optics and the preceding results apply to these waves. They also appear in nonelectromagnetic waves, for instance, acoustic waves, seismic waves, etc. Propagation always generates caustics.

Optical caustics are now understood as Lagrangian singularities and, as singularities, their interest is not restricted to optics. They became indispensable for understanding other domains of mathematical physics, for instance, the variational calculus, the classical mechanics, the Hamilton–Jacobi equations, the control theory, the field theory, etc.

See also: Billiards in Bounded Convex Domains; Normal Forms and Semiclassical Approximation; Stationary Phase Approximation; Singularity and Bifurcation Theory.

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Optimal Cloning of Quantum States

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Introduction

According to the well-known "no-cloning theorem" (Wootters and Zurek 1982) perfect copying of quantum information is impossible, that is, there is no machine which takes a quantum system in an unknown state as input and produces two systems of the same kind, such that none of them is distinguishable from the input by a statistical experiment. In this qualitative form, however, the theorem is not very useful, because in the presence of noise classical information cannot be copied perfectly as well. Therefore, the crucial point is that even under ideal conditions the errors produced in the clones cannot be made arbitrarily small. The best we can hope for is to find an optimal cloning device which makes these errors as small as possible.

More generally, we can consider cloning devices, which take as input a certain number, N, of identically prepared systems, and produce a larger number, M, of systems as output. Again, the cloning task is to make the output state resemble as much as possible a state of M systems all prepared in the same state as the inputs. This variant of the problem is of interest as a "quantum amplifier." It also has a better chance of reasonable success than a cloning device operating on single-input systems: in the limit of many-input systems, the device can make a good statistical estimate of the input density matrix and hence produce arbitrarily good clones.

Figures of Merit

To get a precise mathematical description of the problem, let us consider a one-particle Hilbert space $\mathcal{H}$ (which is assumed to be finite dimensional, $\mathcal{H} = \mathbb{C}^d$, if nothing else is explicitly stated) and the algebras $\mathcal{B}(\mathcal{H}^{\otimes N}), \mathcal{B}(\mathcal{H}^{\otimes M})$ of (bounded) operators on the N-fold, respectively M-fold, tensor product of $\mathcal{H}$. A quantum operation which takes N particles as input and produces M output particles is then described, in the Heisenberg picture, by a completely positive, unital map (a completely positive, unital and normal map if $\mathcal{H}$ is infinite dimensional):

$$T : \mathcal{B}(\mathcal{H}^{\otimes M}) \rightarrow \mathcal{B}(\mathcal{H}^{\otimes N}) \qquad [1]$$

while the Schrödinger picture representation is given in terms of the (pre-)dual of T, that is,

$$T_* : \mathcal{B}_*(\mathcal{H}^{\otimes N}) \rightarrow \mathcal{B}_*(\mathcal{H}^{\otimes M}) \qquad [2]$$

where $\mathcal{B}_*(\cdot)$ denotes the space of trace-class operators. Hence, if T operates on input systems in the (joint) state $\rho^{\otimes N}$, the output systems (i.e., the "clones") are in the state $T_*(\rho^{\otimes N})$. We will call each such T a cloning map.

Now our aim is to find an operation T such that the output state $T_*(\rho^{\otimes N})$ approximates the product state $\rho^{\otimes M}$ as well as possible. The quality of the approximation is measured by a distance function δ on the convex set $\mathcal{S}(\mathcal{H}^{\otimes M}) \subset \mathcal{B}_*(\mathcal{H}^{\otimes M})$ of density operators on $\mathcal{H}^{\otimes M}$ and, since it is impossible to minimize $\delta(T_*(\rho^{\otimes N}), \rho^{\otimes M})$ for all ρ simultaneously, we are looking only for the worst case. Hence, the quality of a cloning map T is measured by a figure of merit of the form

$$\Delta_{X,\delta}(T) = \sup_{\rho \in X} \delta\big(T_*(\rho^{\otimes N}), \rho^{\otimes M}\big) \qquad [3]$$

Here $X \subset \mathcal{S}(\mathcal{H})$ is a set of "preferred" density operators whose role will be explained in the next section. An optimal cloning device is described by a cloning map $\hat{T}$ which minimizes $\Delta_{X,\delta}$, that is,

$$\Delta_{X,\delta}(\hat{T}) \leq \Delta_{X,\delta}(T) \qquad [4]$$

should hold for each cloning map T.

The Preferred Set of States

The set $X \subset \mathcal{S}(\mathcal{H})$ of density operators introduced in the last equation describe *a priori* knowledge about the one-particle input state ρ; for example, if we want to clone only signal states $\rho_1, \ldots, \rho_k$ used to transmit classical information through a quantum channel, the choice for X is $\{\rho_1, \ldots, \rho_k\}$. Other possibilities include: $X = S(\mathcal{H})$ if nothing is known about ρ, the set of pure states, the states in the "equatorial plane" of the Bloch sphere, or Gaussian states if $\mathcal{H}$ is infinite dimensional. Each different choice for X leads to a different variant of the cloning problem, and we will summarize the most relevant cases treated in the literature in the section "Examples."

A different kind of *a priori* knowledge is *a priori* measures, that is, instead of knowing that all possible input states lie in a special set X, we know for each measurable set $X \subset \mathcal{S}(\mathcal{H})$ the probability $\mu(X)$ for $\rho \in X$. Such a situation typically arises when we are trying to clone states of systems which

originate from a source with known characteristics. In this case, we can use mean errors,

$$\bar{\Delta}_{\mu,\delta}(T) = \int_{\mathcal{S}(\mathcal{H})} \delta\big(T^*(\rho^{\otimes N}),\ \rho^{\otimes M}\big)\mu(\mathrm{d}\rho) \qquad [5]$$

as a figure of merit. Sometimes these are easier to compute than maximal errors as in eqn [3]. Often, however, Δ leads to stronger results than $\bar{\Delta}$, therefore we will concentrate our discussion on maximal rather than mean errors.

The Distance Measure

The remaining freedom in eqn [3] is the distance measure δ and there are mainly two physically different choices: we can either check the quality of each clone separately or we can test, in addition, the correlations between output systems. The most common choice for a figure of merit for the first type is given by (where $\hat{\mathrm{tr}}_j$ denotes partial trace over all but the jth tensor factor)

$$\Delta_1(T) = \sup_{\rho\in X,j} \big|1 - \mathcal{F}\big(\hat{\mathrm{tr}}_j T_*(\rho^{\otimes N}),\ \rho\big)\big| \qquad [6]$$

Here $\mathcal{F}(\rho,\sigma)$ denotes the (quadratic) fidelity of ρ and σ, that is,

$$\mathcal{F}(\rho,\sigma) = \mathrm{tr}\Big(\big(\rho^{1/2}\sigma\rho^{1/2}\big)^{1/2}\Big)^2 \qquad [7]$$

and the supremum is taken over all $\rho\in X$ and $j=1,\ldots,N$. Δ_1 measures the worst one-particle error of the output state $T^*(\sigma^{\otimes N})$, and we will refer to it in the following as the local error. If we are interested in correlations too, we have to choose

$$\Delta_{\mathrm{all}}(T) = \sup_{\rho\in X} \big|1 - \mathcal{F}\big(T_*(\rho^{\otimes N}),\rho^{\otimes M}\big)\big| \qquad [8]$$

Δ_{all} measures again a "worst-case" error, but now of the full output with respect to M uncorrelated copies of the input ρ. We will call it the global error. Alternative figures of merit arise if we replace the fidelity in eqns [6] and [8] by other distance measures like the trace norm, the Hilbert–Schmidt norm, or the relative entropy. If X consists only of pure states, the operations T which minimize Δ_1 or Δ_{all} are usually not altered by such different choices. If X is a set of mixed states, however, the correct choice is unclear and might depend on the precise physical context (there is, in particular, no reason to prefer fidelities).

General Properties

Before we consider more special examples in the next section, let us discuss some general properties of the figure of merit $\Delta_{X,\delta}$ from eqn [3] and the corresponding optimization problem.

Existence of Solutions

If the distance measure δ is continuous in the first argument, the optimization problem [4] has a solution, that is, optimal cloning machines exist: the set $\mathcal{T}$ of cloning maps [1] is compact and the quantity $\Delta_{X,\delta}$ is – as a supremum over continuous functions – lower-semicontinuous. Hence, the statement follows from the fact that a lower-semicontinuous function on a compact set always admits a minimizer.

This argument can be generalized to the infinite-dimensional case, if we choose the set $\mathcal{T}$ of allowed cloning maps more carefully (the restriction to normal channels proposed above is most probably not sufficient for this purpose) and if we equip it with an appropriate topology. The latter should be weak enough for $\mathcal{T}$ to be compact, and strong enough for $\Delta_{X,\delta}$ to be lower-semicontinuous. A typical choice is the weak*-topology arising from an embedding of $\mathcal{T}$ into the dual of a Banach space (such that we can apply the Banach–Alaoglu Theorem). Detailed studies in this direction are, however, not yet available.

Covariant Cloning Maps

To solve the optimization problem [4] is a difficult and, in many cases, impossible task. However, it can be simplified significantly if X and δ admit a nontrivial symmetry group. Hence, consider again a distance δ which is continuous and convex in its first argument and a closed subgroup G of the group $U(d)$ of unitary operators on $\mathcal{H}=\mathbb{C}^d$, such that

$$UXU^* \subset X,\quad \delta\big(U^{\otimes M}\rho U^{\otimes M*},\, U^{\otimes M}\sigma U^{\otimes M*}\big) = \delta(\rho,\sigma) \qquad [9]$$

hold for all $U\in G$ and $\rho,\sigma\in\mathcal{S}(\mathcal{H}^{\otimes M})$. Then $\Delta_{X,\delta}$ is invariant under the induced G action on the set $\mathcal{T}$ of cloning maps, that is,

$$\Delta_{X,\delta}(\tau_U T) = \Delta_{X,\delta}(T)$$
$$\text{with } (\tau_U T)(A) = U^{\otimes N}T(U^{\otimes M*}AU^{\otimes M})U^{\otimes N*} \qquad [10]$$

holds for all $U\in G$ and all $T\in\mathcal{T}$. Convexity of $\Delta_{X,\delta}$ in T implies (with the Haar measure μ_{H} on G)

$$\Delta_{X,\delta}(\bar{T}) \le \Delta_{X,\delta}(T),\quad \text{with } \bar{T} = \int_G \tau_U(T)\mu_{\mathrm{H}}(\mathrm{d}U) \qquad [11]$$

for all T. Hence, we can replace each cloning map by its group average $\bar{T}$ without sacrificing the

quality of the clones. This implies that $\bar{T}$ is optimal if T is, and, since $\bar{T}$ is G-covariant,

$$\tau_U(\bar{T}) = \bar{T} \quad \forall U \in G \qquad [12]$$

we can conclude, together with the arguments from the last section, that the optimization problem [4] always admits covariant solutions. Similarly, we can show that permutation invariant (sometimes called "symmetric") solutions exist, that is, cloners which do not prefer a particular clone or a particular input system.

This is a very useful result, because the set of covariant and permutation-invariant T is much smaller than the set of all cloning maps, and it can be parametrized in terms of irreducible representations of G and the permutation group. In particular, the case $G = U(d)$ (such a T is often called "universal" because it does not prefer any direction in the Hilbert space $\mathcal{H}$) leads to quite general solutions.

Relationships with Quantum State Estimation

If a procedure to estimate the input state ρ from a measurement on the N-fold system in the joint state $\rho^{\otimes N}$ is given, there is a simple way to produce a cloning machine: we just have to take the estimate $\hat{\rho}$ for the density matrix ρ and prepare $M > N$ systems in the state $\hat{\rho}^{\otimes M}$. If X is finite and estimation (which in this case is called hypothesis testing) is done in terms of a positive operator valued measure $(E_\sigma)_{\sigma \in X}$, $E_\sigma \in \mathcal{B}(\mathcal{H}^{\otimes N})$, the probability to get the estimate $\sigma \in X$ when the input is in the state $\rho^{\otimes N}$ is given by $\mathrm{tr}(E_\sigma \rho^{\otimes N})$. Hence, the cloning map derived from this estimation scheme is given by

$$\tilde{E}_*(\rho^{\otimes N}) = \sum_{\sigma \in X} \mathrm{tr}\big(E_\sigma \rho^{\otimes N}\big) \sigma^{\otimes M} \qquad [13]$$

A generalization to arbitrary X is straightforward, but requires the use of measure theory. It is easy to see that the cloning map $\tilde{E}$ from eqn [13] is in general not optimal, in particular if M is only slightly bigger than N. However, $\tilde{E}$ has the interesting feature that $\Delta_{X,\delta}(\tilde{E})$ depends only on the number of input systems, N, but not on the number of clones, M, we want to produce. This observation leads immediately to the conjecture that $\tilde{E}$ becomes optimal in the limit $M \to \infty$. A general proof is currently not available, in those cases, however, where optimal cloner and estimater can be explicitly calculated for all N and M (i.e., the cases treated in the sections "Universal pure-state cloning" and "Phase-covariant pure-state cloning") the conjecture is true. A more detailed discussion of this problem together with information about its current status can be found on the web at http://www.imaph.tu-bs.de/qi/problems/problems-html.

Examples

In this section, we will discuss concrete examples that arise from different choices of the distance measure δ and the set X of preferred states.

Universal Pure-State Cloning

The most frequently discussed case arises if X is the set of pure states, that is, the input states are pure, but otherwise unknown. Under this condition, it is sufficient to consider the symmetric part $\mathcal{H}_+^{\otimes N}$ of the tensor product $\mathcal{H}^{\otimes N}$, and only cloning maps $T : \mathcal{B}(\mathcal{H}^{\otimes M}) \to \mathcal{B}(\mathcal{H}_+^{\otimes N})$, because only this part affects the local or the global error. A complete solution for arbitrary N, M and all finite-dimensional Hilbert spaces is available for Δ_{all} in Werner (1998) and for Δ_1 in Keyl and Werner (1999). Both cases admit the same (surprisingly simple) unique solution

$$\hat{T}_*(\sigma) = \frac{d[N]}{d[M]} S_M\Big(\sigma \otimes 1^{\otimes(M-N)}\Big) S_M \qquad [14]$$

where S_M is the projection onto the symmetric tensor product $\mathcal{H}_+^{\otimes M}$ and $d[M]$ denotes the dimension of $\mathcal{H}_+^{\otimes M}$. To derive these results, the group-theoretic methods sketched in the section "Covariant cloning maps" are used. The fact that global and local figures of merit are minimized by the same cloning map is surprising and a special feature of pure-state cloning. It implies that correlations and entanglement between the clones does not matter at all.

Phase-Covariant Pure-State Cloning

Consider a fixed basis $|j\rangle$, $j = 0, \ldots, d-1$, in $\mathcal{H}$ and let X be the set of states given by

$$\psi = |0\rangle + \sum_{j=1}^{d-1} e^{i\phi_j} |j\rangle \qquad [15]$$

where the ϕ_j denote arbitrary phases. Obviously, this set is invariant under the set of all unitaries which are diagonal in the given basis (i.e., a maximal torus in $U(d)$). Using the methods outlined in the section "Covariant cloning maps," the corresponding cloning problem is (almost) completely solved in Buscemi *et al.* (2005). For arbitrary $d = \dim \mathcal{H}$, N and all $M = N + dk$, with $k \in \mathbb{N}$ a

cloning map which minimizes global as well as local errors is given in terms of the unitary

$$\hat{U} : \mathcal{H}_+^{\otimes N} \to \mathcal{H}_+^{\otimes M}, \hat{U}|n_0, \ldots, n_d\rangle = |n_0 + k, \ldots, n_d + k\rangle \qquad [16]$$

where $|n_1, \ldots, n_d\rangle, n_j \in \mathbb{N}$, denotes the number basis of $\mathcal{H}^{\otimes N}$ associated with the distinguished basis $|j\rangle$ of $\mathcal{H}$.

Cloning Finitely Many States

If X is a finite set of pure states, a general solution is not available, but there are several important partial results. The easiest situation arises if the elements of X are mutually orthogonal pure states. In this case, ideal cloning is possible in terms of an appropriately chosen unitary. If the states are linearly independent but nonorthogonal, ideal cloning is possible as well if we consider probabilistic cloning machines (Duan and Guo 1998); that is, there is a nonvanishing probability that the machine fails and does not produce any clones at all (this means T is not unital). Optimal cloning (with deterministic operations) of two nonorthogonal qubit states $\rho_j = |\psi_j\rangle\langle\psi_j|$, $j = 1, 2$, is considered for all N, M in (Bruß *et al.* (1998) and Chefles and Barnett (1999)) (using averaged global fidelity as the figure of merit). The crucial observation in this case is that the optimal clones are pure, that is, $T_*(\rho_j^{\otimes N}) = |\Psi_j\rangle\langle\Psi_j|$ and that the Ψ_j lie in the subspace spanned by the (unattainable) ideal clones $\psi_j^{\otimes M}$.

Universal Mixed-State Cloning

$X = \mathcal{S}(\mathcal{H})$ means that absolutely nothing is known *a priori* about the input state ρ. If the distance measure δ is $U(d)$ and permutation invariant (which is the case for all possible choices discussed in the section "The distance measure") the analysis from the section "Covariant cloning maps" shows that a universal and symmetric minimizer exists. An explicit solution, however, is not known, and even the physically most appropriate choice for δ is unclear. In contrast to the pure-state case, this is a serious question, because the set of optimal cloners is, in this case, much more sensitive to changes in δ. In particular, correlations among the clones become crucial, and it is very likely that local and global figures of merit lead to very different solutions. To emphasize this difference, an operation which minimizes only local errors is sometimes called "broadcasting," rather than cloning. A related problem with (at least) partial solutions ("purification") will be discussed in the section "Purification."

Cloning of Gaussian States

If the Hilbert space is infinite dimensional, the restriction to a reasonable small set X of preferred states is crucial, because otherwise the search for minimizers becomes hopeless. A physically relevant class with nice mathematical properties are Gaussian states and in particular coherent states. Cloning of the latter has been studied in Cerf *et al.* (2005) for the case $N = 1$ (and M arbitrary). As in the section "Covariant cloning maps," it can be shown that the search for optimal cloners can be restricted to those which are covariant with respect to phase space translations. This simplifies the problem significantly and leads to the result that the global error is minimized by Gaussian cloning maps, while in the local case the best cloner is non-Gaussian.

Asymmetric Cloning

In all examples discussed up to now, we have considered symmetric cloners, that is, the quality of all clones is measured with equal weight. Alternatively, we can look for asymmetric cloners which produce clones with different quality and ask for the trade-off between them. This problem was first discussed in Cerf (2000) and later in Iblisdir *et al.* (2005). It can be regarded as a constraint optimization problem, where the error of the first $M' < M$ clones should be minimized under the constraint that the error of the rest is bounded by a fixed value. In Iblisdir *et al.* (2005), it is conjectured that for pure input states and local errors the optimal solution to this problem is given by

$$T_*(\sigma) = V^*\left(\sigma \otimes \mathbb{1}^{\otimes(M-N)}\right)V \qquad [17]$$

where V is a linear combination of projections in the commutant of $\{U^{\otimes N} \mid U \in U(\mathcal{H})\}$. This conjecture is true (at least) for qubits in the case $1 \to n + 1$ and $1 \to 1 + n$.

Related Problems

Instead of cloning, we can also try to approximate other impossible machines by channels which operate on multiple inputs. To this end, we only have to replace the figure of merit [6] by

$$\Delta_{1,\beta}(T) = \sup_{\rho \in X, j} \left|1 - \mathcal{F}\left(\hat{\mathrm{tr}}_j T_*(\rho^{\otimes N}),\ \beta(\rho)\right)\right| \qquad [18]$$

where $\beta : \mathcal{S}(\mathcal{H}) \to \mathcal{S}(\mathcal{H})$ is a (possibly nonlinear) functional which describes the task we want to approximate. The generalization $\Delta_{\mathrm{all},\beta}$ of Δ_{all} can be given similarly. If β has the appropriate continuity and symmetry properties, the discussion in the section "General properties" applies completely, that is, we can assume covariance and permutation

invariance, and we can consider operations which use state estimation in an intermediate step.

Purification

Consider N quantum systems, all originally prepared in the same pure state σ, and then subsequently exposed to the same (known) decoherence process, described by a depolarizing channel R. The task of purification is to produce M output systems which approximate the original pure input state as well as possible. Hence, the corresponding figure of merit arises with $X = \{R(\sigma) \mid \sigma \text{ pure}\}$ and $\beta(\rho) = R^{-1}(\rho)$. This problem is discussed for qubits in Cirac *et al.* (1999), Keyl and Werner (2001) and D'Ariano *et al.* (2005). The optimal purifier can be given explicitly for all N, M in terms of irreducible SU(2) representations. Surprisingly, it turns out that the output purity can be improved even if the number of outputs, M, is larger than the number of available input systems, N (although N should be large enough). If we measure purity in terms of local errors, it can be shown that, in the limit $N \to \infty$, perfectly purified qubits can be produced at an infinite rate (i.e., the number of output systems per input system can become infinite). However, we have to pay for this result with extremely large correlations between the output systems. Therefore, the global error does not disappear asymptotically, if we insist on a nonvanishing rate.

Universal Not

"Universal not" (UNOT) is an operation which sends each pure state σ to its orthocomplement. This is a positive but not a completely positive operation. Hence, it cannot be performed by any physical device. However, we can try to approximate it by a cloning map T operating on N input systems. The corresponding figure of merit [18] arises if X is the set of pure states and $\beta(\rho) = \mathbb{1} - \rho$. In Bužek *et al.* (1999), it is shown that the optimal solution to this problem (for all N and M) is to estimate and reprepare as described in the section "Relationships with quantum state estimation." Approximating UNOT is, therefore, significantly more difficult than (pure-state) cloning, where the optimal solution is always (for finite M) better than estimation.

See also: Channels in Quantum Information Theory; Compact Groups and Their Representations; Positive Maps on C^*-algebras.

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Optimal Transportation

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The purpose of this article is to introduce some of the main ideas of optimal transportation theory. A lot more can be found in Villani's book (Villani 2003), in a somewhat similar spirit. Supplementary information is also available in Ambrosio *et al.* (2005), Evans and Gangbo (1999), and Rüschendorf and Rachev (1990).

Transportation Maps

Let us start by a rather abstract definition:

Definition 1 Let X and Y be two topological spaces with Borel probability measures α and β, respectively. We say that a Borel map $T : X \to Y$ is a transportation map between (X, α) and (Y, β) if, for each Borel subset A of Y,

$$\int_{T(x)\in A} \alpha(\mathrm{d}x) = \int_{y\in A} \beta(\mathrm{d}y)$$

It is customary to say that T pushes forward α to β, or to say that β is the image of α by T. An abstract measure-theoretic result asserts that there is always such a transportation map T, as soon as α has no atom (i.e., the α measure of any point $x \in X$ is zero).

A more concrete situation is when $X = \bar{\Omega}_0$, $Y = \bar{\Omega}_1$, where Ω_0 and Ω_1 are two smooth bounded open subsets of the d-dimensional Euclidean space $\boldsymbol{R}^d$. In such a case, a classical result, due to Moser and improved by Dacorogna and Moser (1990), reads:

Theorem 1 *Let Ω_0 and Ω_1 be two smooth bounded open sets in $\boldsymbol{R}^d$. Let $\rho_0 > 0$ and $\rho_1 > 0$ be two smooth functions on $\boldsymbol{R}^d$ such that*

$$\int_{\Omega_0} \rho_0(x)\mathrm{d}x = \int_{\Omega_1} \rho_1(x)\mathrm{d}x = 1$$

Then there is a smooth transportation map T between $(\bar{\Omega}_0, \rho_0(x)\mathrm{d}x)$ and $(\bar{\Omega}_1, \rho_0(y)\mathrm{d}y)$. Furthermore, T is an orientation-preserving diffeomorphism and solves the Jacobian equation:

$$\rho_1(T(x)) \det(DT(x)) = \rho_0(x), \quad \forall x \in \Omega_0 \qquad [1]$$

Transportation Maps with Convex Potentials

An important property of Moser's construction, which we did not state, is the possibility of prescribing the restriction of T along the boundary $\partial\Omega_0$. If one does not care about this latter property, one can improve Theorem 1 as follows (Caffarelli 1992):

Theorem 2 *Assume further that Ω_1 is a uniformly strictly convex set. Then, there is a transportation map T with a smooth convex potential, namely*

$$T(x) = D\Phi(x), \quad \forall x \in \Omega_0$$

for some smooth convex function Φ defined on $\boldsymbol{R}^d$ and strictly convex on Ω_0. In addition, among all Borel maps T transporting $(\bar{\Omega}_0, \rho_0(x)\mathrm{d}x)$ to $(\bar{\Omega}_1, \rho_1(y)\mathrm{d}y)$, $D\Phi$ is the unique map that minimizes

$$\inf_T \int_{\boldsymbol{R}^d} |T(x) - x|^2 \rho_0(x)\mathrm{d}x \qquad [2]$$

where $|\cdot|$ denotes the Euclidean norm on $\boldsymbol{R}^d$.

Because of its characterization, $T = D\Phi$ is often called the "optimal transportation map" with respect to the "transportation cost" [2]. Notice that, because of the Jacobian equation [1], Φ automatically is a classical solution to the Monge–Ampère equation:

$$\rho_1(D\Phi(x)) \det(D^2\Phi(x)) = \rho_0(x), \quad \forall x \in \Omega_0 \qquad [3]$$

(The Monge–Ampère equation is a famous geometric PDE, related to the seeking of hypersurfaces with prescribed Gaussian curvature.) The main gain with respect to Moser's construction is the property that the optimal map T has, at each $x \in \Omega_0$, a Jacobian matrix $DT(x) = D^2\Phi(x)$ which is a positive-definite symmetric matrix. This property has been first exploited by McCann (1997) and later by many authors (see Villani (2003), for many references) to prove a large series of geometric and functional inequalities. A very fine example can be found in Barthe (1998). Let us just consider, as an elementary illustration, a short and sharp proof of the isoperimetric inequality using the optimal transportation map.

A Proof of the Isoperimetric Inequality Using Optimal Transportation Maps

Let us recall the isoperimetric inequality:

Theorem 3 *Let Ω be a smooth bounded open subset in $\boldsymbol{R}^d$. Then*

$$|\partial\Omega| \geq \mathrm{d}|B_1|^{1/d}|\Omega|^{1-1/d}$$

holds true where B_1 is the unit ball in $\boldsymbol{R}^d$, $|\Omega|$ and $|\partial\Omega|$, respectively, denote the d-dimensional volume of Ω and the $(d-1)$-dimensional Hausdorff measure of the boundary $\partial\Omega$. In addition, the inequality becomes an equality if and only if Ω is a ball.

To prove this result, let us define densities:

$$\rho_0(x) = \frac{1}{|\Omega|}, \quad x \in \Omega$$
$$\rho_1(y) = \frac{1}{|B_1|}, \quad y \in B_1$$

and consider the associated optimal transportation map $D\Phi$ from $(\bar{\Omega}_0, \rho_0(x)\mathrm{d}x)$ to $(\bar{\Omega}_1, \rho_0(y)\mathrm{d}y)$. From the Monge–Ampère equation,

$$\rho_1(D\Phi(x)) \det(D^2\Phi(x)) = \rho_0(x)$$

we get:

$$\det(D^2\Phi(x)) = \frac{|B_1|}{|\Omega|}, \quad x \in \Omega \qquad [4]$$

Since the range of $D\Phi$ on Ω is the unit ball B_1, we have

$$I = \int_{\partial\Omega} D\Phi(x) \cdot n(x)\mathrm{d}\sigma(x) \leq \int_{\partial\Omega} \mathrm{d}\sigma(x) = |\partial\Omega|$$

where $n(x)$ and $\mathrm{d}\sigma(x)$ respectively, denote the outward unit normal and the $(d-1)$-dimensional

Hausdorff measure along $\partial\Omega$. Using the divergence theorem, we also have:

$$I = \int_\Omega \Delta\Phi(x)\mathrm{d}x$$

where $\Delta\Phi(x) = \mathrm{trace}(D^2\Phi(x))$ is the Laplacian of Φ. From the geometric mean inequality, we know that, for any symmetric matrix $A \geq 0$,

$$(\det A)^{1/d} \leq 1/d \text{ trace } (A)$$

holds true, with equality if and only if A is equal to the identity matrix multiplied by a non-negative scalar factor. Thus,

$$\begin{aligned} I &\geq d \int_\Omega (\det(D^2\Phi(x))^{1/d}\mathrm{d}x \\ &= d|\Omega|^{1-1/d}|B_1|^{1/d} \end{aligned}$$

(because of [4]). So, we have obtained the isoperimetric inequality:

$$|\partial\Omega| \geq \mathrm{d}|B_1|^{1/d}|\Omega|^{1-1/d}$$

Let us now consider the case when this inequality becomes an equality. Then, necessarily, for each $x \in \Omega, A = D^2\Phi(x)$ satisfies $\det A = (\mathrm{trace}(A)/d)^d$ and, therefore, must be the identity matrix multiplied by a scalar factor $\lambda > 0$, possibly depending on x. Because of [4], the determinant of $D^2\Phi(x)$ is constant over Ω. Thus, $\lambda > 0$ must be constant. It follows that $D\Phi(x) = \lambda(x - a)$, for some point a in $\mathbf{R}^d$. Therefore, Ω must be the ball centered at a of radius $1/\lambda$.

Monge's Optimal Transportation Problem

Theorem 2 is one of the numerous avatars of the so-called optimal transportation theory that goes back to Monge's mass transfer problem which addressed in 1781 the 'mémoire sur la théorie des déblais et des remblais' and was completely renewed by Kantorovich in the 1940s (see e.g., Rüschendorf and Rachev (1990) for instance). Let us quote a typical result, similar to Theorem 2, but without regularity assumptions on the data (see Brenier and Caffarelli (1992)):

Theorem 4 *Let ρ_0 be a non-negative Lebesgue integrable function on $\mathbf{R}^d$, such that*

$$\int_{\mathbf{R}^d} \rho_0(x)\mathrm{d}x = 1$$

Then for any Borel probability measure $\rho_1(\mathrm{d}y)$ with compact support on $\mathbf{R}^d$, there is a unique map T transporting $\rho_0(x)\mathrm{d}x$ to $\rho_1(\mathrm{d}y)$, which minimizes

$$\int_{\mathbf{R}^d} |T(x) - x|^2 \rho_0(x)\mathrm{d}x$$

where $|\cdot|$ denotes the Euclidean norm on $\mathbf{R}^d$. In addition, there is a Lipschitz continuous convex function Φ defined on $\mathbf{R}^d$ such that $T(x) = D\Phi(x)$ for ρ_0 almost every $x \in \mathbf{R}^d$, which implies:

$$\int_{\mathbf{R}^d} f(D\Phi(x))\rho_0(x)\mathrm{d}x = \int_{\mathbf{R}^d} f(y)\rho_1(\mathrm{d}y)$$

for all continuous functions f on $\mathbf{R}^d$.

Theorem 2, which can be interpreted as a regularity result with respect to Theorem 4, is the main output of Caffarelli's regularity theory for transportation maps with convex potentials (Caffarelli 1992). Caffarelli's analysis starts by a proof that Φ actually is a weak solution of the Monge–Ampère equation [3] in the sense of Alexandrov and is strictly convex. Then, Caffarelli shows that $D^2\Phi$ is Hölder continuous, as soon as ρ_0 and ρ_1 are Hölder continuous.

Notice that the convexity assumption for Ω_1 is crucial to insure the regularity of the convex potential. Caffarelli provided counter-examples when Ω_1 is made of two separate balls attached together by a sufficiently thin pipe.

Surprisingly enough, results such as Theorem 4 are related to concrete applications in, for example, astrophysics, image processing, etc. (Frisch *et al.* 2002, Haker and Tannenbaum 2003).

The Kantorovich Optimal Transportation Problem

The Monge optimal transportation problem can be solved using the Kantorovich duality method, based on the key concept of "generalized transportation maps," also called "transportation plans" or "doubly stochastic measures." The abstract definition is:

Definition 2 Let X and Y be two topological spaces with Borel probability measures α and β, respectively. We say that a Borel probability measure μ on $X \times Y$ is a generalized transportation map, or a transportation plan, if its marginals are, respectively, α and β, namely

$$\begin{aligned} \int_{x\in A, y\in Y} \mu(\mathrm{d}x, \mathrm{d}y) &= \int_{x\in A} \alpha(\mathrm{d}x) \\ \int_{x\in X, y\in B} \mu(\mathrm{d}x, \mathrm{d}y) &= \int_{y\in B} \beta(\mathrm{d}y) \end{aligned} \qquad [5]$$

for all Borel subsets A and B of X and Y, respectively.

The Monge–Kantorovich (MK) optimal transportation problem amounts, given a "transportation

cost," that is, a continuous function $c: X \times Y \to \boldsymbol{R}$, to find a minimizer for

$$I_{\mathrm{MK}} = \inf_{\mu} \int c(x, y)\mu(\mathrm{d}x, \mathrm{d}y) \qquad [6]$$

where μ is subject to be a transportation plan between (X, α) and (Y, β). Notice that this problem is convex (and can be seen as an infinite-dimensional linear program) and its dual problem can be easily computed (using, e.g., Rockafellar's theorem in convex analysis and assuming, for simplicity, that both X and Y are compact).

Theorem 5 *We have*

$$I_{\mathrm{MK}} = \sup_{a,b}\left\{ \int a(x)\alpha(\mathrm{d}x) + \int b(y)\beta(\mathrm{d}y) \right\} \qquad [7]$$

where (a, b) *is any pair of continuous functions, defined on X and Y, respectively, and subject to*:

$$a(x) + b(y) \le c(x, y), \quad \forall x \in X, \forall y \in Y$$

Of course, each transportation map T, in the sense of Definition 1, can be seen as a transportation plan μ in the Kantorovich framework, just by setting

$$\mu(\mathrm{d}x, \mathrm{d}y) = \delta(y - T(x))\alpha(\mathrm{d}x)$$

which means

$$\int_{x \in A, y \in B} \mu(\mathrm{d}x, \mathrm{d}y) = \int_{x \in A, T(x) \in B} \alpha(\mathrm{d}x)$$

for all Borel subsets A and B of X and Y, respectively. Then, we have

$$\int c(x, y)\mu(\mathrm{d}x, \mathrm{d}y) = \int c(x, T(x))\alpha(\mathrm{d}x)$$

So, the MK problem can be seen as a "relaxed" version of the "classical" optimal transportation problem à *la* Monge:

$$I_{\mathrm{M}} = \inf_{T} \int c(x, T(x))\alpha(\mathrm{d}x) \qquad [8]$$

where T is subject to be a transportation map between (X, α) and (Y, β). Indeed, we have $I_{\mathrm{MK}} \le I_{\mathrm{M}}$. It turns out that, in many important situations, there is no gap between these two values, which makes the MK problem a perfectly convenient convex substitute for the original, nonconvex, Monge transportation problem. This is, in particular, the case of the situation considered in Theorem 4, when the cost function is just

$$c(x, y) = |x - y|^2$$

or, more generally, $c(x, y) = k(x - y)$, where k is a uniformly strictly convex function. A typical result is:

Theorem 5 *Let* ρ_0 *be a non-negative Lebesgue integrable function on* $\boldsymbol{R}^d$*, with unit integral, and* $\rho_1(\mathrm{d}y)$ *be a Borel probability measure with compact support on* $\boldsymbol{R}^d$*. Let k be a uniformly strictly convex function on* $\boldsymbol{R}^d$*. Then the MK problem*

$$I_{\mathrm{MK}} = \inf_{\mu} \int k(y - x)\mu(\mathrm{d}x, \mathrm{d}y)$$

where μ *is subject to be a transportation plan between* $\rho_0(x)\mathrm{d}x$ *and* $\rho_1(\mathrm{d}y)$ *on* $\boldsymbol{R}^d$*, has a unique solution of form*

$$\mu(\mathrm{d}x, \mathrm{d}y) = \delta(y - T(x))\alpha(\mathrm{d}x)$$

where T is the unique minimizer of the Monge problem:

$$I_{\mathrm{M}} = \inf_{T} \int k(T(x) - x)\rho_0(x)\mathrm{d}x$$

among all transportation maps T between $\rho_0(x)\mathrm{d}x$ *and* $\rho_1(\mathrm{d}y)$ *on* $\boldsymbol{R}^d$*. In addition* $I_{\mathrm{MK}} = I_{\mathrm{M}}$.

Proof for Theorem 5 (Sketch) For simplicity, we assume that ρ_0 and ρ_1 are both compactly supported in a ball B in $\boldsymbol{R}^d$ and we limit ourselves to the simplest cost function $k(x) = |x|^2/2$. We first denote by M the set of all Borel regular probability measures ν on $B \times B$ having $\rho_0(x)\mathrm{d}x$ and $\rho_1(\mathrm{d}y)$ as marginals, which means

$$\int_{B \times B} f(x)\nu(\mathrm{d}x, \mathrm{d}y) = \int_B f(x)\rho_0(x)\mathrm{d}x$$

$$\int_{B \times B} f(y)\nu(\mathrm{d}x, \mathrm{d}y) = \int_B f(y)\rho_1(\mathrm{d}y)$$

for all continuous functions f on $\boldsymbol{R}^d$. From Theorem 7, we deduce:

$$\max_{\nu \in M} \int_{B \times B} x \cdot y\nu(\mathrm{d}x, \mathrm{d}y) = \inf \int_B [\Phi(x)\rho_0(x) + \Psi(x)\rho_1(x)]\mathrm{d}x$$

where the infimum is taken over all pairs (Φ, Ψ) of continuous functions on B satisfying

$$\Phi(x) + \Psi(y) \ge x \cdot y, \quad \forall x \in B, \forall y \in B$$

Then, it can be established that the infimum is attained by a pair (Φ, Ψ) such that Φ is the restriction of a Lipschitz continuous convex function defined on $\boldsymbol{R}^d$, and for $\rho_0(x)\mathrm{d}x$ almost every point of $\boldsymbol{R}^d$, Ψ coincides with the Legendre–Fenchel transform of Φ,

$$\mathrm{LF}(\Phi)(y) = \sup_{x \in \boldsymbol{R}^d}(x \cdot y - \Phi(x))$$

Moreover, if $\nu = \nu_{\text{opt}} \in M$ maximizes $\int_{B\times B} x \cdot y \nu(\mathrm{d}x, \mathrm{d}y)$, then

$$\Phi(x) + \Psi(y) = x \cdot y$$

holds for ν_{opt}-almost every $(x, y) \in \boldsymbol{R}^d \times \boldsymbol{R}^d$. Using well-known properties of the Legendre–Fenchel transform in convex analysis, one deduces that ν_{opt} is necessarily of the form

$$\nu_{\text{opt}}(\mathrm{d}x, \mathrm{d}y) = \delta(y - D\Phi(x))\rho_0(x)\,\mathrm{d}x$$

which implies

$$\int_{\boldsymbol{R}^d \times \boldsymbol{R}^d} f(y)\nu_{\text{opt}}(\mathrm{d}x, \mathrm{d}y) = \int_{\boldsymbol{R}^d} f(D\Phi(x))\rho_0(x)\,\mathrm{d}x$$

for all continuous functions f on $\boldsymbol{R}^d$ and achieves the proof since the second marginal of ν_{opt} is $\rho_1(\mathrm{d}y)$.

The Wasserstein Distance

Optimal transportation theory is strongly related to the geometric analysis of probability measures. For simplicity, let us just consider the space Prob(B) of all Borel probability measures ρ supported by some fixed ball B in $\boldsymbol{R}^d$. This space is compact for the weak topology of measures. An equivalent definition of this topology is provided by the distance d, naturally attached to the MK problem:

$$\mathrm{d}(\rho_0, \rho_1) = \inf_{\nu} \left(\int_{B\times B} |x - y|^2 \mu(\mathrm{d}x, \mathrm{d}y) \right)^{1/2} \qquad [9]$$

where μ is subject to be a transportation plan between ρ_0 and ρ_1 on B. (Of course, more general convex functions k can be used to define the cost function.) It has become popular to call this distance as Wasserstein distance (or its generalizations for various k). It turns out that Prob(B) equipped with this distance has a formal Riemannian structure (Otto 2001, Ambrosio *et al.* 2005). For instance, given two probability measures $\rho_0(x)\mathrm{d}x$ and $\rho_1(x)\mathrm{d}x$, we can define a "shortest path" $t \to \rho(t, \cdot) \in$ Prob(B) such that $\rho(0) = \rho_0, \rho(1) = \rho_1$, just by setting:

$$\rho(t, \mathrm{d}x) = \int_B \delta(a + (D\Phi(a) - a)t - x)\rho_0(a)\mathrm{d}a, \quad \forall t \in [0, 1]$$

where $D\Phi$ is the optimal transportation map between ρ_0 and ρ_1 on B. This idea, which is somewhat related to the geometric analysis of hydrodynamics and various concepts of generalized flows Arnol'd and Khesin 1998, Brenier, was successfully used by McCann (1997) and Otto (2001). In particular, the concept of convexity along these geodesic paths on Prob(B) has been pointed out by McCann (1997) to be a crucial tool for new proofs of geometric and functional inequalities. Otto, and other contributors (see Ambrosio *et al.* (2005) for a comprehensive discussion), observed that many important parabolic or dissipative evolution PDEs can be described as "gradient flows" (or "steepest descent") of such functionals, with respect to the Wasserstein metric.

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Ordinary Special Functions

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Introduction

The exponential function, the logarithm, the trigonometric functions, and various other functions are often used in mathematics and physics. They are transcendental functions in the sense that they cannot be obtained by a finite number of operations as a solution of an algebraic (polynomial) equation. Typically, they are obtained by a Taylor series expansion. Many other higher transcendental functions arise in mathematical physics, often as solutions of differential equations. A precise knowledge of the behavior of such functions, their relation with other functions, addition, multiplication and composition properties, representations as an infinite series, or as an integral, often shed a lot of light onto the problem in which they arise. If they are sufficiently useful to a large audience, then they usually get a name and they will be called special functions. In what follows, we describe a few of these special functions of one variable, but clearly this is just a tip of the iceberg. Many other special functions exist and we refer to the classical tables of Abramowitz and Stegun (1964) and the Bateman manuscript project (Erdélyi *et al.* 1953–55) for more special functions. Nowadays, there have been numerous q-extensions of special functions (*see* q-Special Functions).

Gamma and Beta Function

The gamma function is defined by

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt, \quad \Re z > 0. \qquad [1]$$

It satisfies the functional equation $\Gamma(z+1) = z\Gamma(z)$ and since $\Gamma(1) = 1$ we have $\Gamma(n+1) = n!$ for $n \in \mathbb{N}$. The gamma function therefore extends the factorial function for integers to complex numbers. The functional equation

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z} \qquad [2]$$

allows to continue the gamma function analytically to $\Re z < 0$ and the gamma function becomes an analytic function in the complex plane, with a simple pole at 0 and at all the negative integers. The residue of $\Gamma(z)$ at $z = -n$ is equal to $(-1)^n/n!$. Legendre's duplication formula is

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}} \Gamma(z)\Gamma(z+1/2) \qquad [3]$$

from which one can obtain the special value $\Gamma(1/2) = \sqrt{\pi}$. Finally, two useful infinite product representations are

$$\Gamma(z) = \lim_{n\to\infty} \frac{n! n^z}{z(z+1)\cdots(z+n)}$$

and

$$\frac{1}{\Gamma(z)} = z e^{\gamma z} \prod_{n=1}^{\infty} \left((1 + z/n) e^{-z/n} \right)$$

where γ is Euler's constant:

$$\gamma = \lim_{n\to\infty} \left(\sum_{k=1}^{n} \frac{1}{k} - \log n \right) = 0.577\,215\,664\,9\ldots \qquad [4]$$

The beta function is a function of two variables given by

$$B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\, dt \qquad \Re x > 0, \Re y > 0 \qquad [5]$$

Clearly it satisfies $B(x,y) = B(y,x)$ and it is related to the gamma function by

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \qquad [6]$$

The gamma and beta function are quite useful in probability theory. One of the most common probability distributions on the positive real line is the gamma distribution

$$\Pr(X \le x) = \frac{1}{\beta^\alpha \Gamma(\alpha)} \int_0^x e^{-t/\beta} t^{\alpha-1}\, dt, \quad x \ge 0$$

The case $\alpha = 3/2$ is the Maxwell–Boltzmann distribution. The most common probability distribution on the interval [0, 1] is the beta distribution

$$\Pr(Y \le x) = \frac{1}{B(\alpha,\beta)} \int_0^x t^{\alpha-1}(1-t)^{\beta-1} dt$$

where $0 \le x \le 1$.

The psi function is the logarithmic derivative of the gamma function

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} \qquad [7]$$

It is meromorphic with simple poles at 0 and at the negative integers. Special values are $\psi(1) = -\gamma$ and

$$\psi(n+1) = \sum_{k=1}^{n} \frac{1}{k} - \gamma$$

where γ is Euler's constant. These can be obtained from the functional equation

$$\psi(z) = \psi(z+1) - \frac{1}{z}$$

Bessel Functions

Bessel's differential equation is

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0 \qquad [8]$$

where derivatives are with respect to x and ν is a complex number. This differential equation has a regular singularity at $x=0$ and an irregular singularity at $x=\infty$. The standard method of finding a solution in the neighborhood of a regular singularity gives the solution

$$J_\nu(x) = (x/2)^\nu \sum_{k=0}^{\infty} \frac{(-x^2/4)^k}{k!\Gamma(k+\nu+1)}$$

and $J_{-\nu}(x)$ is another solution (if $\nu \neq 0$). The function J_ν is called the "Bessel function of the first kind" and ν is the "order" of the Bessel function. The series $x^{-\nu}J_\nu(x)$ is an entire function of the variable x. The function

$$Y_\nu(x) = \frac{J_\nu(x)\cos(\nu\pi) - J_{-\nu}(x)}{\sin(\nu\pi)}$$

is also a solution of Bessel's differential equation and is known as the "Bessel function of the second kind of order ν." Two other solutions that are often used are

$$H_\nu^{(1)}(x) = J_\nu(x) + \mathrm{i}Y_\nu(x)$$
$$H_\nu^{(2)}(x) = J_\nu(x) - \mathrm{i}Y_\nu(x)$$

which are the first and second "Hankel functions."

Bessel functions appear if one solves the wave equation in cylindrical or spherical coordinates, using separation of variables. The Helmholtz equation $\nabla^2 F + k^2 F = 0$ in cylindrical coordinates ρ, ϕ, z is

$$\frac{\partial^2 F}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial F}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 F}{\partial \phi^2} + \frac{\partial^2 F}{\partial z^2} + k^2 F = 0$$

and if we look for a solution of the form $f(\rho)g(\phi)h(z)$, then this leads to a differential equation for f of the form

$$\frac{\mathrm{d}^2 f}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}f}{\mathrm{d}\rho} + [k^2 - a^2 - (\nu/\rho)^2]f = 0$$

where a and ν are separation constants. The general solution is $f(\rho) = Z_\nu(\rho(k^2 - a^2))$, where Z_ν is any of the Bessel functions given higher or linear combinations of them. In spherical coordinates r, θ, ϕ the Helmholtz equation is

$$\frac{\partial^2 F}{\partial r^2} + \frac{2}{r}\frac{\partial F}{\partial r} + \frac{1}{r^2}\frac{\partial^2 F}{\partial \theta^2} + \frac{\cot\theta}{r^2}\frac{\partial F}{\partial \theta} + \frac{1}{r^2 \sin^2\phi}\frac{\partial^2 F}{\partial \phi^2} + k^2 F = 0$$

and for a solution of the form $f(r)g(\theta)h(\phi)$ one obtains a differential equation for f of the form

$$\frac{1}{r}\frac{\mathrm{d}^2(rf)}{\mathrm{d}r^2} + [k^2 - \nu(\nu+1)/r^2]f = 0$$

with general solution $f(r) = Z_{\nu+(1/2)}(kr)/\sqrt{r}$.

Bessel functions have very simple differentiation formulas:

$$[z^\nu J_\nu(z)]' = z^\nu J_{\nu-1}(z)$$
$$[z^{-\nu} J_\nu(z)]' = -z^{-\nu} J_{\nu+1}(z)$$

The first formula can be seen as a lowering operation, the second as a raising operation. Some integral representations are

$$J_\nu(z) = \frac{(z/2)^\nu}{\sqrt{\pi}\,\Gamma(\nu+1/2)} \int_0^\pi \sin^{2\nu}\theta \cos(z\cos\theta)\mathrm{d}\theta$$

or

$$J_\nu(z) = \frac{(z/2)^\nu}{\sqrt{\pi}\,\Gamma(\nu+1/2)} \int_{-1}^{1} (1 - x^2)^{\nu - 1/2} \cos zx \, \mathrm{d}x$$

which hold for $\Re\nu > -1/2$. For real ν the Bessel function J_ν has infinitely many real zeros, and when $\nu > -1$, then all the zeros are real. All the zeros are simple (except possibly at the origin). Each of the functions $J_\nu(z), Y_\nu(z), H_\nu^{(1)}(z)$, or $H_\nu^{(2)}(z)$ satisfies the recurrence relation

$$za_{\nu-1}(z) + za_{\nu+1}(z) = 2\nu a_\nu(z)$$

and the differential–recurrence relation

$$a_{\nu-1}(z) - a_{\nu-1}(z) = 2a'_\nu(z)$$

Modified Bessel Functions

The modified Bessel equation is

$$x^2y'' + xy' - (x^2 + \nu^2)y = 0 \qquad [9]$$

Clearly $J_\nu(ix)$ is a solution of this equation. The "modified Bessel function of the first kind" is defined as

$$I_\nu(x) = e^{-\nu\pi i/2}J_\nu(xe^{\pi i/2}), \quad -\pi < \arg x \le \pi/2 \qquad [10]$$

so that

$$I_\nu(x) = (x/2)^\nu \sum_{k=0}^{\infty} \frac{(x/2)^{2k}}{k!\Gamma(\nu + k + 1)}$$

If ν is not an integer, then $I_\nu(x)$ and $I_{-\nu}(x)$ are two linearly independent solutions of [9], and when $\nu = n$ is an integer one has $I_n(x) = I_{-n}(x)$. The "modified Bessel function of the second kind" is defined by

$$K_\nu(x) = \frac{\pi}{2\sin\nu\pi}[I_{-\nu}(x) - I_\nu(x)]$$

Some special cases of modified Bessel functions are

$$I_{1/2}(x) = \sqrt{\frac{2}{\pi x}}\sinh x$$

$$I_{-1/2}(x) = \sqrt{\frac{2}{\pi x}}\cosh x$$

and

$$K_{1/2}(x) = \sqrt{\frac{\pi}{2x}}e^{-x}$$

One has the integral representation

$$K_\nu(z) = \int_0^\infty e^{-z\cosh x}\cosh \nu x \, dx$$

and

$$I_\nu(z) = \frac{(z/2)^\nu}{\sqrt{\pi}\Gamma(\nu + 1/2)}\int_{-1}^{1}(1 - x^2)^{\nu - 1/2}e^{\pm zx}\,dx$$

whenever $\Re\nu > -1/2$. The "Airy functions" are given by

$$\mathrm{Ai}(z) = \frac{\sqrt{z}}{3}\left[I_{-1/3}(\zeta) - I_{1/3}(\zeta)\right] = \frac{\sqrt{z/3}}{\pi}K_{1/3}(\zeta)$$

$$\mathrm{Bi}(z) = \sqrt{z/3}\left[I_{-1/3}(\zeta) + I_{1/3}(\zeta)\right]$$

where $\zeta = 2z^{2/3}/3$. They are both a solution of Airy's differential equation

$$y''(z) - zy(z) = 0$$

Hypergeometric Series

A power series $\sum_{n=0}^{\infty} c_n z^n$ is said to be hypergeometric when the ratio c_{n+1}/c_n is a rational function of the index n. Most series that one finds in calculus textbooks are hypergeometric series and some of them define important special functions. When

$$\frac{c_{n+1}}{c_n} = \frac{(n + a_1)(n + a_2)\cdots(n + a_p)}{(n + b_1)(n + b_2)\cdots(n + b_q)(n + 1)}$$

then we write the corresponding series as

$$ {}_pF_q\left(\begin{matrix} a_1, a_2, \ldots, a_p \\ b_1, b_2, \ldots, b_q \end{matrix}\middle| z\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n(a_2)_n\cdots(a_p)_n}{(b_1)_n(b_2)_n\cdots(b_q)_n}\frac{z^n}{n!} \qquad [11]$$

where $(a)_n = a(a+1)(a+2)\cdots(a+n-1)$, with $(a)_0 = 1$, is the rising factorial or Pochhammer symbol. When p and q are small, one also uses the notation ${}_pF_q(a_1, \ldots, a_p; b_1, \ldots, b_q; z)$ where a semicolon (;) is used to separate the parameters in the numerator from the parameters in the denominator and also to separate the parameters from the variable z. Some special cases are:

- the exponential series

$$ {}_0F_0(-;-;z) = \sum_{n=0}^{\infty}\frac{z^n}{n!} = \exp(z)$$

- the geometric series

$$ {}_1F_0(1;-;z) = \sum_{n=0}^{\infty} z^n = \frac{1}{1-z}$$

- the binomial series

$$ {}_1F_0(-\alpha;-;-z) = \sum_{n=0}^{\infty}\binom{\alpha}{n}z^n = (1+z)^\alpha$$

- the logarithmic function

$$ {}_2F_1(1,1;2;z) = \sum_{n=0}^{\infty}\frac{z^n}{n+1} = -\frac{1}{z}\log(1-z)$$

- the Bessel function

$$(z/2)^\nu {}_0F_1(-;\nu+1;-z^2/4) = \Gamma(\nu+1)J_\nu(z)$$

For generic values of the parameters, we see that the hypergeometric series converges everywhere in the complex plane when $q \ge p$, it converges for $|z| < 1$ when $p = q + 1$, and for $p > q + 1$ it is only defined at

$z = 0$. When one of the numerator parameters is a negative integer, say $a_1 = -m$, then the series is terminating and defines a polynomial of degree m. None of the denominator parameters is allowed to be a negative integer $-m$, unless there is a numerator parameter which is a negative integer $-k$ with $k < m$. For $q \geq p$, the hypergeometric series therefore defines an entire function which is the corresponding hypergeometric function. For $p = q + 1$, the hypergeometric series only converges in the open unit disk, but sometimes it can be continued analytically to a larger domain in the complex plane. The analytic continuation of the hypergeometric series is then called the hypergeometric function. Take for example the geometric series, then it is clear that the hypergeometric series converges in the open unit disk, but the corresponding hypergeometric function is defined in the whole complex plane with a simple pole at $z = 1$. The logarithmic function $-\log(1-z)$ has a hypergeometric series in the open unit disk, but it can be continued analytically to the complex plane with a cut along $[1, \infty)$ and a branch point at $z = 1$.

Gauss Hypergeometric Function

The most famous hypergeometric function is the Gauss hypergeometric function defined for $|z| < 1$ by the hypergeometric series

$$ {}_2F_1(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n n!} z^n \qquad [12] $$

which is often denoted by $F(a, b; c; z)$. It is a solution of the hypergeometric equation

$$ z(1-z)y''(z) + [c - (a+b+1)z]y'(z) - aby(z) = 0 \qquad [13] $$

and this solution is regular at $z = 0$. Obviously, ${}_2F_1(a, b; c; z) = {}_2F_1(b, a; c; z)$. The six functions ${}_2F_1(a \pm 1, b; c; z)$, ${}_2F_1(a, b \pm 1; c; z)$, and ${}_2F_1(a, b; c \pm 1; z)$ are called contiguous to ${}_2F_1(a, b; c; z)$ and there are 15 linear relations (with coefficients which are linear functions of z) between ${}_2F_1(a, b; c; z)$ and any two contiguous functions. Two of these relations are

$$ (2a - c - az + bz)F(a, b; c; z) + (c - a)F(a-1, b; c; z) + a(z-1)F(a+1, v; c; z) = 0 $$

and

$$ c(a - (c-b)z)F(a, b; c; z) - ac(1-z)F(a+1, b; c; z) + (c-a)(c-b)zF(a, b; c+1; z) = 0 $$

Euler gave the integral representation

$$ {}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{x^{b-1}(1-x)^{c-b-1}}{(1-zx)^a} \mathrm{d}x \qquad [14] $$

for $\Re c > 0$ and $\Re b > 0$. This allows to find the analytic continuation from the open unit disk to the complex plane. A useful result is the Gauss summation formula

$$ {}_2F_1(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} $$
$$ \Re(c-a-b) > 0 $$

The special case for a terminating series is known as the Chu–Vandermonde sum

$$ {}_2F_1(-n, a; c; 1) = \frac{(c-a)_n}{(c)_n} $$

Pfaff's transformation is

$$ {}_2F_1(a, b; c; z) = (1-z)^{-a} {}_2F_1\left(a, c-b; c; \frac{z}{z-1}\right) $$

and Euler's transformation is

$$ {}_2F_1(a, b; c; z) = (1-z)^{c-a-b} {}_2F_1(c-a, c-b; c; z) $$

Confluent Hypergeometric Function

The hypergeometric series ${}_1F_1(a; c; z)$ defines an entire function in the complex plane and satisfies the differential equation

$$ zy''(z) + (c-z)y'(z) - ay(z) = 0 \qquad [15] $$

This hypergeometric series (and the differential equation) are formally obtained from ${}_2F_1(a, b; c; z/b)$ by letting $b \to \infty$, which gives a confluence of two of the singularities at $z = \infty$. This is the reason why the differential equation [15] is known as the confluent hypergeometric equation. The solution

$$ \Phi(a, c; z) = {}_1F_1(a; c; z) \qquad [16] $$

is called a confluent hypergeometric function, and a second linearly independent solution of [15] is $z^{1-c}\Phi(c-a+1, 2-c; z)$. The function

$$ \Psi(a, c; z) = \frac{\Gamma(1-c)}{\Gamma(a-c+1)} \Phi(a, c; z) + \frac{\Gamma(c-1)}{\Gamma(a)} z^{1-c} \Phi(a-c+1, 2-c; z) \qquad [17] $$

is therefore also a solution of eqn [15]. The following integral representations hold:

$$\Phi(a, c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 e^{zx} x^{a-1}(1-x)^{c-a-1} dx$$

whenever $\Re c > \Re a > 0$, and

$$\Psi(a, c; z) = \frac{1}{\Gamma(a)} \int_0^\infty e^{-zx} x^{a-1}(1+x)^{c-a-1} dx$$

whenever $\Re a > 0$.

The "Whittaker functions" are defined as

$$M_{\lambda,\mu}(z) = e^{-z/2} z^{c/2} \Phi(a, c; z)$$
$$W_{\lambda,\mu}(z) = e^{-z/2} z^{c/2} \Psi(a, c; z)$$

with $\lambda = -a + c/2$ and $\mu = (c-1)/2$. They are a solution of the Whittaker equation

$$y''(z) + \left(-\frac{1}{4} + \frac{\lambda}{z} + \frac{1-4\mu^2}{4z^2}\right) y(z) = 0$$

The "parabolic cylinder functions" are also confluent hypergeometric functions. They are given by

$$\begin{aligned} D_\nu(z) &= 2^{\nu/2} e^{-z^2/4} \Psi(-\nu/2, 1/2; z^2/2) \\ &= 2^{(\nu-1)/2} e^{-z^2/4} z \Psi((1-\nu)/2, 3/2; z^2/2) \end{aligned}$$

When ν is a non-negative integer, one finds Hermite polynomials

$$H_n(z) = 2^{n/2} e^{z^2/2} D_n(\sqrt{2}z)$$

Classical Orthogonal Polynomials

A family of polynomials $\{p_n(x), n \in \mathbb{N}\}$, where p_n has degree n, is orthogonal on the real line if there is a positive measure μ on the real line for which

$$\int_{\mathbb{R}} p_n(x) p_m(x) d\mu(x) = h_n \delta_{m,n} \qquad [18]$$

Usually the measure μ is absolutely continuous, in which case $d\mu(x) = w(x)\, dx$ with w a non-negative density function on the real line, or μ is discrete and supported on a finite or at most countable set. Any family of orthogonal polynomials satisfies a "three-term recurrence relation"

$$x p_n(x) = A_n p_{n+1}(x) + B_n p_n(x) + C_n p_{n-1}(x) \qquad [19]$$

with $C_n A_{n-1} > 0$ for every $n \geq 1$. For the monic polynomials $P_n(x) = p_n(x)/k_n$, with $k_n = 1/(A_0 A_1 A_2 \cdots A_{n-1})$ this relation becomes

$$P_{n+1}(x) = (x - b_n) P_n(x) - a_n^2 P_{n-1}(x)$$

with $b_n = B_n$ and $a_n^2 = A_{n-1} C_n$. This recurrence relation gives rise to a tridiagonal matrix

$$J = \begin{pmatrix} b_0 & a_1 & 0 & 0 & 0 & 0 \\ a_1 & b_1 & a_2 & 0 & 0 & 0 \\ 0 & a_2 & b_2 & a_3 & 0 & 0 \\ 0 & 0 & a_3 & b_3 & a_4 & 0 \\ 0 & 0 & 0 & a_4 & \ddots & \ddots \\ 0 & 0 & 0 & 0 & \ddots & \end{pmatrix}$$

which is formally symmetric and which is called the "Jacobi matrix." The spectral measure of this operator, acting on $\ell_2(\mathbb{N})$, is equal to the orthogonality measure μ whenever this symmetric operator can be extended to a self-adjoint operator. If this is not possible in a unique way – a situation which can occur for unbounded operators only – then every self-adjoint extension of J gives rise to a spectral measure which can be used for the orthogonality conditions [18]. In this case, there are infinitely many positive measures which can be used in the orthogonality relations and all these measures have the same moments

$$m_n = \int_{\mathbb{R}} x^n \, d\mu(x)$$

Some families of orthogonal polynomials have additional properties which are quite useful in many practical and physical applications, such as the following:

- The derivatives p_n' are again a family of orthogonal polynomials (Hahn property).
- The polynomials p_n satisfy a second-order linear differential equation of the form

  $$\sigma(x) y''(x) + \tau y'(x) = \lambda_n y(x)$$

  where σ is a polynomial of degree at most 2, τ is a polynomial of degree 1, both independent of n, and λ_n is a real number (Bochner property).
- The polynomials can be obtained by a Rodrigues formula

  $$w(x) p_n(x) = C_n \frac{d^n}{dx^n} (w(x) \sigma^n(x))$$

  where w is a non-negative function and σ a polynomial of degree at most 2 (Hildebrand property).

There are three families of orthogonal polynomials on the real line which have these three properties, and

each of these three properties characterizes these families. These are the Hermite polynomials, the Laguerre polynomials, and the Jacobi polynomials. In a more general situation when the orthogonality relation is described by a linear functional and the functional is not required to be positive, one has an additional family of Bessel polynomials. The densities $w(x)$ for these families all satisfy a first-order differential equation $[\sigma(x)w(x)]' = \tau(x)w(x)$, where σ is a polynomial of degree at most 2 and τ a polynomial of degree 1. This equation is known as the "Pearson equation."

Hermite Polynomials

Hermite polynomials $H_n(x)$ are orthogonal with respect to the normal density $w(x) = e^{-x^2}$:

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2}\,dx = 2^n n!\delta_{n,m}$$

Observe that the density satisfies $w' = -2xw$ so that $\sigma = 1$ and $\tau(x) = -2x$. The recurrence relation is

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

and the polynomials satisfy the second-order differential equation

$$y''(x) - 2xy'(x) + 2ny(x) = 0$$

The functions $h_n(x) = e^{-x^2/2}H_n(x)$ satisfy the differential equation

$$h_n''(x) + (2n + 1 - x^2)h_n(x) = 0$$

The derivatives satisfy $H_n'(x) = 2nH_{n-1}(x)$ (lowering operation) and one also has $[e^{-x^2}H_n(x)]' = -e^{-x^2} H_{n+1}(x)$ (raising operation). The Rodrigues formula is

$$e^{-x^2}H_n(x) = (-1)^n \frac{d^n}{dx^n}e^{-x^2}$$

The polynomials can be written as a hypergeometric series

$$H_n(x) = (2x)^n {}_2F_0(-n/2, -(n-1)/2; -; -1/x^2)$$

or alternatively as

$$H_n(x) = n! \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k (2x)^{n-2k}}{k!(n-2k)!}$$

Their generating function is

$$\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \exp(2xt - t^2)$$

Hermite polynomials are relevant for the analysis of the quantum harmonic oscillator, and the lowering and raising operators there correspond to creation and annihilation.

Laguerre Polynomials

Laguerre polynomials $L_n^\alpha(x)$ are for $\alpha > -1$ orthogonal with respect to the gamma density $w(x) = x^\alpha e^{-x}$ on $[0, \infty)$:

$$\int_0^\infty L_n^\alpha(x)L_m^\alpha(x)x^\alpha e^{-x}\,dx = \frac{\Gamma(n+\alpha)}{n!}\delta_{m,n}$$

The Pearson equation is $[xw]' = (\alpha + 1 - x)w$ so that $\sigma(x) = x$ and $\tau(x) = \alpha + 1 - x$. The recurrence relation is

$$(n+1)L_{n+1}^\alpha(x) = (2n + \alpha + 1 - x)L_n^\alpha(x) - (n+\alpha)L_{n-1}^\alpha(x)$$

and the differential equation is

$$xy''(x) + (\alpha + 1 - x)y'(x) + ny(x) = 0$$

The functions $\ell_n(x) = x^{\alpha/2}e^{-x/2}L_n^\alpha(x)$ satisfy

$$(x\ell_n')' + \left(n + \frac{\alpha+1}{2} - \frac{x}{4} - \frac{\alpha^2}{4x}\right)\ell_n = 0$$

Differentiation has the effect that

$$[L_n^\alpha(x)]' = -L_{n-1}^{\alpha+1}(x)$$

and

$$[x^\alpha e^{-x}L_n^\alpha(x)]' = (n+1)x^{\alpha-1}e^{-x}L_{n+1}^{\alpha-1}(x)$$

The Rodrigues formula is

$$x^\alpha e^{-x}L_n^\alpha(x) = \frac{1}{n!}\frac{d^n}{dx^n}[x^{n+\alpha}e^{-x}]$$

The hypergeometric expression is

$$n!L_n^\alpha(x) = (\alpha+1)_n {}_1F_1(-n; \alpha+1; x)$$

and the generating function is

$$\sum_{n=0}^{\infty} L_n^\alpha(x)t^n = (1-t)^{-\alpha-1}\exp\left(\frac{xt}{t-1}\right)$$

Laguerre polynomials occur as eigenfunctions of the hydrogen atom.

Jacobi Polynomials

Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ are orthogonal for the beta density $w(x) = (1-x)^\alpha(1+x)^\beta$ on $[-1,1]$ whenever $\alpha > -1$ and $\beta > -1$:

$$\int_{-1}^{1} P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x)(1-x)^\alpha(1+x)^\beta \, dx = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)}\delta_{n,m}$$

The Pearson equation is $[(1-x^2)w]' = [\beta-\alpha-(\alpha+\beta+2)x]w$ and the differential equation is

$$(1-x^2)y''(x) + [\beta-\alpha-(\alpha+\beta+2)x]y'(x) + n(n+\alpha+\beta+1)y(x) = 0$$

Differentiation has the effect

$$\left[P_n^{(\alpha,\beta)}(x)\right]' = (n+\alpha+\beta+1)/2P_{n-1}^{(\alpha+1,\beta+1)}(x)$$

and

$$\left[(1-x)^\alpha(1+x)^\beta P_n^{(\alpha,\beta)}(x)\right]' = -2(n+1)(1-x)^{\alpha-1}(1+x)^{\beta-1}P_{n+1}^{(\alpha-1,\beta-1)}(x)$$

The Rodrigues formula is

$$(1-x)^\alpha(1+x)^\beta P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}\left[(1-x)^{n+\alpha}(1+x)^{n+\beta}\right]$$

In terms of hypergeometric series, one has

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+1)_n}{n!} \times {}_2F_1\left(\begin{matrix}-n, n+\alpha+\beta+1\\ \alpha+1\end{matrix}\,\middle|\,\frac{1-x}{2}\right)$$

Observe that one has $P_n^{(\alpha,\beta)}(-x) = (-1)^n P_n^{(\beta,\alpha)}(x)$.

Special cases of the Jacobi polynomials are as follows:

- The "Legendre polynomials" $P_n(x) = P_n^{(0,0)}(x)$. They appear when the Laplacian is separated in spherical coordinates as functions of the polar angle θ, for which $x = \cos\theta$.
- The "Chebyshev polynomials" of the first kind

  $$T_n(x) = P_n^{(-1/2,-1/2)}(x)/P_n^{(-1/2,-1/2)}(1)$$

  and of the second kind

  $$U_n(x) = (n+1)P_n^{(1/2,1/2)}(x)/P_n^{(1/2,1/2)}(1)$$

  These functions are more easily written by using the change of variable $x = \cos\theta$ and then $T_n(\cos\theta) = \cos n\theta$ and $U_n(\cos\theta) = \sin(n+1)\theta/\sin\theta$.
- The "Gegenbauer polynomials" or ultraspherical polynomials are Jacobi polynomials with equal parameters:

  $$C_n^\lambda(x) = (2\lambda)_n/(\lambda+1/2)_n P_n^{(\lambda-1/2,\lambda-1/2)}(x)$$

Gegenbauer polynomials are involved in the angular or spatial part of the wave function of physical systems in a central potential in both position and momentum space, and in the spatial part of the wave function of hydrogenic systems in momentum space, as well as in the eigenfunctions of several quantum-mechanical potentials, such as the relativistic harmonic oscillator.

Other Classical Orthogonal Polynomials

Instead of restricting attention to the differential operator $D = d/dx$, one can also use the (forward) difference operator Δ for which $\Delta f(x) = f(x+1) - f(x)$, the divided difference operator Δ_λ for which $\Delta_\lambda f(x) = \Delta f(\lambda(x))/\Delta\lambda(x)$ with a quadratic function λ, or certain q-difference operators and look for orthogonal polynomials that satisfy difference equations in the variable x. Together with the three-term recurrence relation (in the degree n), one then has families of polynomials satisfying a bispectral problem. For the difference operator and the divided difference operator, this gives several important families of orthogonal polynomials which all have a hypergeometric representation. These hypergeometric polynomials are usually listed in a table, and each level indicates the number of parameters and/or the order of the hypergeometric function. This table is known as Askey's table and is given in **Figure 1**. The extension with q-difference operators involves basic hypergeometric series and q-extensions of classical orthogonal polynomials.

"Charlier polynomials" $C_n(x;a)$ are orthogonal with respect to the Poisson distribution

$$\sum_{k=0}^{\infty} C_n(k;a)C_m(k;a)\frac{a^k}{k!} = e^a/a^n\delta_{n,m}$$

The recurrence relation is

$$aC_{n+1}(x;a) + (x-n-a)C_n(x;a) + nC_{n-1}(x;a) = 0$$

and the second-order difference equation is

$$ay(x+1) + (n-x-a)y(x) + xy(x-1) = 0$$

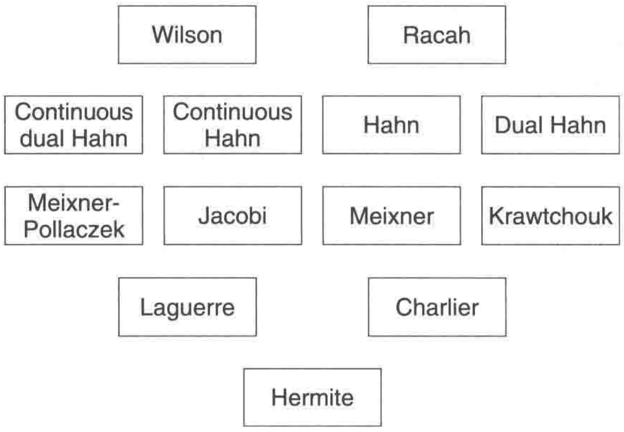


Figure 1 Askey's table.

The forward difference operator has the effect $\Delta C_n(x;a) = -n/aC_{n-1}(x;a)$ and the backward difference operator $\nabla f(x) = f(x) - f(x-1)$ has the effect $\nabla[a^x/x!C_n(x;a)] = a^x/x!C_{n+1}(x;a)$. The hypergeometric representation is $C_n(x;a) = {}_2F_0(-n - x; -; -1/a)$. Observe that the variable x appears as a parameter of the hypergeometric series.

"Krawtchouk polynomials" $K_n(x;p,N)$ are orthogonal with respect to the binomial distribution:

$$\sum_{k=0}^{N} K_n(k;p,N)K_m(k;p,N)\binom{N}{k}p^k(1-p)^{N-k} = \frac{(-1)^n n!}{(-N)_n}p^{-n}(1-p)^n\delta_{n,m}$$

where N is a positive integer and $0 < p < 1$. They are given by $K_n(x;p,N) = {}_2F_1(-n,\ -x;\ -N;1/p)$ and correspond to Meixner polynomials for which the parameter β is a negative integer.

"Meixner polynomials" $m_n(x;\beta,c)$ are orthogonal with respect to the negative binomial distribution (Pascal distribution)

$$\sum_{k=0}^{\infty} m_n(k;\beta,c)m_j(k;\beta,c)\frac{(\beta)_k c^k}{k!} = \frac{n!}{c^n(\beta)_n(1-c)^\beta}\delta_{n,j}$$

where $\beta > 0$ and $0 < c < 1$. They are given by $m_n(x;\beta,c) = {}_2F_1(-n,\ -x;\beta;1-1/c)$.

"Meixner–Pollaczek polynomials" $P_n^\lambda(x;\phi)$ are orthogonal on $(-\infty,\infty)$:

$$\int_{-\infty}^{\infty} P_m^\lambda(x;\phi)P_n^\lambda(x;\phi)e^{(2\phi-\pi)x}|\Gamma(\lambda+ix)|^2\,dx = \frac{2\pi\Gamma(n+2\lambda)}{(2\sin\phi)^{2\lambda}n!}\delta_{m,n}$$

where $\lambda > 0$ and $0 < \phi < \pi$. The appropriate difference operator δ has an imaginary shift $\delta f(x) = f(x+i/2) - f(x-i/2)$ and one has $\delta P_n^\lambda(x;\phi) = 2\sin\phi P_{n-1}^{\lambda+1/2}(x;\phi)$. They are given by

$$P_n^\lambda(x;\phi) = \frac{(2\lambda)_n}{n!}e^{in\phi}{}_2F_1\left(\left.\begin{matrix}-n,\lambda+ix\\2\lambda\end{matrix}\right|1-e^{-2i\phi}\right)$$

"Hahn and dual Hahn polynomials" are orthogonal on a finite set of points. Hahn polynomials are given by

$$Q_n(x;\alpha,\beta,N) = {}_3F_2\left(\left.\begin{matrix}-n,n+\alpha+\beta+1,-x\\\alpha+1,-N\end{matrix}\right|1\right)$$

and their orthogonality is with respect to a hypergeometric distribution on $\{0,1,\ldots,N\}$. The appropriate difference operator is the (forward) difference operator Δ. They are related to the $3-j$ symbols or Wigner coefficients that arise when considering angular momenta in two quantum systems. Dual Hahn polynomials are given by

$$R_n(\lambda(x);\gamma,\delta,N) = {}_3F_2\left(\left.\begin{matrix}-n,-x,x+\gamma+\delta+1\\\gamma+1,-N\end{matrix}\right|1\right)$$

where $\lambda(x) = x(x+\gamma+\delta+1)$. They are obtained from the Hahn polynomials by interchanging the roles of n and x. They are orthogonal on the set $\{\lambda(0),\lambda(1),\ldots,\lambda(N)\}$. The appropriate difference operator is the divided difference operator which acts on f as $\Delta f(\lambda(x))/\Delta\lambda(x)$.

"Continuous Hahn and dual Hahn polynomials" are orthogonal on the real line. The continuous Hahn polynomials are

$$p_n(x;a;b;c;d) = i^n\frac{(a+c)_n(a+d)_n}{n!} \times {}_3F_2\left(\left.\begin{matrix}-n,n+a+b+c+d-1,a+ix\\a+c,a+d\end{matrix}\right|1\right)$$

and the appropriate difference operator is the difference operator δ with imaginary shift. The continuous dual Hahn polynomials are

$$S_n(x^2;a,b,c) = (a+b)_n(a+c)_n \times {}_3F_2\left(\left.\begin{matrix}-n,a+ix,a-ix\\a+b,a+c\end{matrix}\right|1\right)$$

and the appropriate difference operator is the divided difference operator which acts on f as $\delta f(x^2)/\delta x^2$.

"Wilson polynomials" are the most general system of hypergeometric polynomials satisfying a bispectral problem. All the other classical orthogonal polynomials can be obtained from them by taking

appropriate parameters or as limiting cases. They are given by

$$\frac{W_n(x^2;a,b,c,d)}{(a+b)_n(a+c)_n(a+d)_n} = {}_4F_3\left(\begin{matrix}-n,n+a+b+c+d-1,a+\mathrm{i}x,a-\mathrm{i}x\\ a+b,a+c,a+d\end{matrix}\middle|1\right)$$

and for $\Re(a,b,c,d)>0$ (with nonreal parts appearing in conjugate pairs) they are orthogonal on the positive real line with respect to the weight function

$$w(x)=\left|\frac{\Gamma(a+\mathrm{i}x)\Gamma(b+\mathrm{i}x)\Gamma(c+\mathrm{i}x)\Gamma(d+\mathrm{i}x)}{\Gamma(2\mathrm{i}x)}\right|$$

"Racah polynomials" can be obtained from Wilson polynomials when the parameters are such that one of $a+b$, $a+c$, or $a+d$ is a negative integer $-N$. They are given by

$$R_n(\lambda(x);\alpha,\beta,\gamma,\delta) = {}_4F_1\left(\begin{matrix}-n,n+\alpha+\beta+1,-x,x+\gamma+\delta+1\\ \alpha+1,\beta+\delta+1,\gamma+1\end{matrix}\middle|1\right)$$

where $\alpha+1=-N$ or $\beta+\delta+1=-N$ or $\gamma+1=-N$, and N is a non-negative integer. They are orthogonal on the finite set $\{\lambda(0),\lambda(1),\ldots,\lambda(N)\}$, where $\lambda(x)=x(x+\gamma+\delta+1)$. They arise as $6-j$ symbols in the coupling of three angular momenta.

See also: Combinatorics: Overview; Compact Groups and their Representations; Integrable Systems: Overview; Painlevé Equations; q-Special Functions; Random Matrix Theory in Physics; Separation of Variables for Differential Equations.

Further Reading

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◎编辑手记

世界著名数学家、哲学家、逻辑学家弗雷格曾给出了一个著名等式：半个数学家＋半个哲学家＝好的哲学家＋好的数学家.他解释说："一个好的数学家，至少是半个哲学家；一个好的哲学家，至少是半个数学家."

本书的目的就是要用物理学家替换上述等式中的哲学家.

举两个刚刚读到的例子，从中可见物理学家对数学也会有贡献.物理学家李政道和杨振宁在研究统计力学的一个问题时，遇到了一类特殊的多项式

$$P(z)=\sum_{j=0}^{m}a_j z^j$$

的集合$\mathscr{P}$.他们能够分析出，$\mathscr{P}$中的任意一个多项式P的所有根都位于复平面的单位圆周$\{z:|z|=1\}$上.因此他们猜测这个结论对$\mathscr{P}$中的所有多项式P都成立.如果他们可以找到一个酉矩阵$\boldsymbol{U}$使得$P(z)$是$\boldsymbol{U}$的特征多项式，即$P(z)=\det(z\boldsymbol{I}-\boldsymbol{U})$，那么猜想就证明了.这是任何一个学过高等数学的人都会想到的办法，但这个方法在此不管用.杨和李有很好的数学功底，因此找到一个证明，但这个证明并不简单.现在有更容易的证明了，这要特别归功于浅野太郎(Taro Asano).为证明杨一李单位圆定理(将在下面陈述)，我们需要将单变量z的m次多项式P替换为m个变量$z_1,\cdots,z_m$的多项式$Q(z_1,\cdots,z_m)$，$Q(z_1,\cdots,z_m)$关于每个变量z_i都是一次的.我们感兴趣的是这样一类多项式$Q(z_1,\cdots,z_m)$的集合$\mathcal{Q}$：只要$|z_1|<1,\cdots,|z_m|<1$就有$Q(z_1,\cdots,z_m)\neq 0$.因此，如果$P(z)=Q(z,\cdots,z)$且在$\mathcal{Q}$中，则P的根ξ满足$|\xi|\geqslant 1$.(在我们感兴趣的情况下，存在一个对称$z\to z^{-1}$，因此也有$|\xi^{-1}|>1$，从而$|\xi|=1$.)很明显，如果$Q(z_1,\cdots,z_m)$与$\widetilde{Q}(z_{m+1},\cdots,z_{m+n})$在$\mathcal{Q}$中，则

$$Q(z_1,\cdots,z_m)\widetilde{Q}(z_{m+1},\cdots,z_{m+n})$$

也在$\mathcal{Q}$中.我们现在描述一个不那么显然的运算，称之为浅野缩并，它将$\mathcal{Q}$中的多项式变为$\mathcal{Q}$中的多项式.记

$$Q(z_1,\cdots,z_m)=Az_jz_k+Bz_j+Cz_k+D$$

其中A,B,C,D是变量$z_1,\cdots,z_m$中除去z_j,z_k之外的其余$m-2$个变量的多项式.浅野缩并将两个变量z_j,z_k替换为一个单独的变量z_{jk}，使得

$$Az_jz_k+Bz_j+Cz_k+D\to Az_{jk}+D$$

从一个m元多项式Q出发，经过一次浅野缩并，我们得到一个$m-1$元多项式，如果原来的多项式在$\mathcal{Q}$中，则所得的新的多项式也在$\mathcal{Q}$中.(这是一个简单的练习：$Az_{jk}+D$的根是$Az^2+(B+C)z+D$的两根之积的相反数.)可以验证，如果$-1\leqslant a_{jk}\leqslant 1$，则两个变量$z_j,z_k$的形如

$$z_jz_k+a_{jk}(z_j+z_k)+1$$

的多项式也在 Q 中.(令多项式等于零,则得到一个映射 $z_j \to z_k$,该映射是一个对合,并且将单位圆的内部映射到单位圆的外部.)将这些多项式相继相乘,当同一个变量出现两次时做一次浅野缩并,最后令所有的变量都等于 z,则我们得到杨—李单位圆定理:对于实数 $a_{jk}=a_{kj}$,$-1\leqslant a_{jk}\leqslant 1$,多项式

$$P(z)=\sum_{X\subset\{1,\cdots,m\}} z^{|X|}\prod_{j\in X}\prod_{k\notin X}a_{jk} \qquad (*)$$

的所有根都位于单位圆周上①.

再比如物理学家张宗燧.张宗燧步入量子场论研究领域,主要受到玻尔(N. Bohr)的影响.从两人的通信中,可以看出张宗燧对理论研究的偏好.而在理论研究中,张宗燧又有明显的数学倾向.其研究特点为:数学技巧强,善于应用数学解析物理理论问题.在物理研究中,他主张多做群论和对称性的工作.其研究成果中数学计算和表达都相当"清楚、干脆、可靠",结论简明准确.在《数学译林》为田方增先生百岁诞辰的贺信中就提到:泛函分析学科在中国科学院数学研究所几乎一开始就是基础理论与应用并重地发展.按科学规划的精神,从 1958 年起数学所泛函分析学科强调其发展要侧重于与微分方程、物理学、高尖科技和国民经济建设之联系.为此,田方增、关肇直常与吴新谋、张宗燧等合作,使数学所内泛函分析的发展始终注意与微分方程及现代数学物理的联系,先后组织了量子场理论、粒子迁移理论和电磁波理论中数学问题之研究等学术讨论班.他撰写的学术论文为发展中国在这一领域的数学研究做出了重要贡献.田方增与关肇直一起成功地在中国开辟了应用泛函分析的一个重要领域——粒子迁移理论的数学基础及问题的研究.

所以说数学和物理互易性强.一些数学家后来成了物理学家(例如戴森(Freeman Dyson)),而另一些人正好相反(例如钱德拉(Harish Chandra)、博特(Roul Bott)),他们从物理学家变成了数学家.最夸张的莫过于威腾(Edward Witten,1951—).1990 年获得菲尔兹奖的理论物理学家威腾于 1976 年在普林斯顿大学在诺贝尔奖得主(2004)格罗斯(David Gross)的指导下获得物理学博士学位;但他从未获得过数学博士学位.

那么学习物理到底应该掌握多少数学呢?

一位致力于学习理论物理的学生曾请教赫柏林院士怎样治学.赫先生说:"要想搞理论物理,首先数学要好.前两年先把斯米尔诺夫的五卷及变分学、微分几何、数理方法、拓扑和积分等学完,然后开始进入近代数学,要学流形、群、连续群、李群、现代微分几何等."

当然这只是入门级的数学.

本套丛书貌似物理实则充斥着现代数学,正如中国科学院理论物理研究所吴岳良研究员所评介的那样:

本书物理学部分与数学部分的关系很难分开.实际上,经典力学、电磁学、统计力学、量子力学、流体力学、可积系统和动力系统中的许多物理问题可归结为求解数学上的常微分方程、偏微分方程、积分方程、微分积分方程等数学物理方程,物理学问题的解会涉及复变函数和特殊函数等多种函数,在求解时又会用到变分技术、调和分析、泛函分析等各种数学分析方法.同时,对爱因斯坦狭义相对论和广义相对论,它不仅改变了人们的时空观,还使得闵可夫斯基时空的几何学和黎曼空间的几何学成为物理理论的数学基础,同时也使得向量分析、张量分析和微分几何等成为必要的数学分析工具.在量子力学中,物理量成为算子,物理状态用波函数来描述,算子的谱才是测量到的物理量.在量子场论中,波函数又被二次量子化成为算子用来描述基本粒子在相互作用过程中的产生和湮灭.这使得算子代数、量子化方法和路径积分等数学理论和方法成为量子物理的数学基础.粒子物理学家发现自然界的 3 种基本作用力:电磁相互作用、弱相互作用和强相互作用可用规范理论来描述,并完全由规范对称性来支配,这些对称性在数学上用李群和李代数来描写.事实上,晶体的结构也是由欧几里得空间中的转动群来描述,这使得群论在物理学中的应用,尤其在粒子物理中的应用变得越来越重要.在规范理论中,规范势当作基本的量子场,而它被发现就是数学家在现代微分几何学中所研究的纤维丛上的联络,这使得有关纤维丛的拓扑不变量在粒子物理和量子场论研究中变得重要起来,如规范场的磁单极子和瞬子解及手征量子反常等.在量子引力和超弦理论的研究中,不仅运用到已有的数学理论和方法,尤其是现代数学,还促进了数学理论本身的发展.同样,在凝聚态物质和光学方面,物质的拓扑相和拓扑缺陷、拓扑量子计算等也应用到了许多现代数学方法,这使得代数拓扑、代数方法、量子群、复几何、辛几何与拓扑、低维几何、非交换几何等数学理论和数学方法越来越多地渗透到理论物理的研究中.另外,在研究微观物理对象的随机性和各种随机过程的统计规律、无序系统和动力系统时,随机方法和离散数学等也得到越来越广泛

① 见杨振宁,李政道,"Statistical Theory of Equations of State and Phase transition. Ⅱ. Lattice Gas and Ising Model", Phys. Rev. (2) 87(1952),410-419;也见 T. Asano, "Theorems on the partition functions of the Heisenberg feeromagnets", J. Phys. Soc. Japan, 29 (1970),350-359. 长期以来我都为杨—李单位圆定理着迷(见 D. Ruelle, "Extension of the Lee-Yang circle theorem", Phys. Rev. Lett. 26 (1971),303-304),而且我认为在这个领域仍然有未被揭示出的神秘.(2010 年,吕埃勒再次发表了一篇关于杨—李单位圆定理的文章,见 Characterization of Lee-Yang polynomials, *Annals of Mathematics*, 171(2010),589-603.——译者注.)

的应用.

数学对物理的影响有多大?

正如本书前言中所写:

当然,数学是确实存在的.事实上,从某种角度而言,物理学是由精确的数学逻辑所操控的:古希腊人把空间几何结构变成了一种真实的艺术形式.就我所知,古希腊人是"数学物理"的第一个践行者,他们引入了坐标轴的概念,从而把空间几何的所有量都转化为一些简单的数字.今天,这些被称作"物理学的基本定律".直到很久以后我们才认识到如下事实:时间流可以类似地被坐标化,它连同空间一起,同样可用几何方法来解决.于是,有一些疯狂的人对数字的魔力很感兴趣,但是,我们的现实世界似乎确实包含许多超出我们分析能力的地方.

渐渐地,所有这一切都变了.月亮和其他行星的运动好像都满足几何定律.伽利略和牛顿设法去发现这些运动的合乎逻辑的定律,并注意到质量的概念也适用于太空中的物体,就像地球上的苹果和大炮一样,这使得太空更容易被我们所理解.同时人们发现,电子、磁场、光和声音也完全按照数学方程在运转.

科学家认为:开展对"数学物理"的深入研究,有助于揭示出物理学与数学之间的内在联系.事实上,从自然哲学发展到物理学,除了使用实验手段和新的思维方法,数学起了不可替代的作用.当人们通过分析大量实验数据和吸取各种唯象理论的精髓,以严格的数学语言和简洁的数学公式描述支配物质基本结构和宇宙演化的物理规律时,物理学的简洁美、统一美、对称与不对称美则通过深刻的数学美反映出来.可以说,自从物理学成为自然科学的一门独立学科后,物理学与数学之间的关系变得密不可分.古代的许多科学家既是数学家也是物理学家,尤其到了近代和现代,许多理论物理学家对数学的运用和发展起到了更为积极的推进作用,数学家和理论物理学家之间的合作也变得越来越频繁、越来越深入,他们成为了"数学物理"的践行者.大家最为熟知的古希腊的阿基米德,他既是著名的数学家也是著名的物理学家,他很早就利用数学这个工具证明了杠杆原理和浮力原理,并做了大量的实验.牛顿在研究物体和天体的运动规律时发展出新的数学方法——微积分.爱因斯坦则运用对当时的物理学家来说全新的数学方法——微分几何和黎曼几何,创立了广义相对论.爱因斯坦曾回忆说:"1912年我突然认识到,高斯的曲面理论是解开这个秘密的钥匙,他的曲面坐标系意义重大.不过,当时我还不知道黎曼已经更深入地研究了几何基础.我突然想起,读大学时盖泽先生给我们上的几何就包括高斯理论……我认识到几何基础具有物理学意义.当我从布拉格回到苏黎世时,我亲爱的朋友、数学家格罗斯曼也在苏黎世.他告诉了我高斯,然后是黎曼.格罗斯曼两肋插刀,直接催生广义相对论."

伟大的几何学家海曼·格拉斯曼①在1844年发表的《Lineale Ausdehnungslehre》(《延拓理论》).这本书像麦比乌斯的那本名著一样具有丰富的思想,但与麦的写作风格不同,非常晦涩,以至几十年未被人注意,也没有被人读懂,只是在其他书和文章中出现了一系列类似的思想之后,才认识到这些思想出自格拉斯曼的书,不过为时已晚.如果你想领略一下这种抽象的笔法,你只要看一下这本书里的某几章的标题,如:"纯数学之概念之导出""延拓理论之推导""延拓理论之叙述""表示之形式""一般形式理论之概述".你只有费劲地钻通了这些内容之后才接触到所述内容的纯抽象的表示,不过仍然很难读懂.直到1862年该书出版了后期的修订本②,格拉斯曼才用了一种比较容易接受的表示法,即坐标表示法.此外,格拉斯曼选了一个词——Ausdehnungslehre(延拓论),用以暗示他的研究可应用于任意维空间,而几何学对他而言只不过是这个完全抽象的新学科在普通三维空间中的应用.但是他造的这个新词并没有生根,人们现今简称为"n维几何学".

我们普通读者可能易将数学物理与数学物理方程相混淆,其实这是两个内涵和外延都不同的概念,后者只能视为前者的一个真子集,而前者不论从内容上还是所涵盖的范围都远远超过了后者,但有一点共同之处是它们的问题都源自于物理,但解决都来自于数学家.比如迪利克雷猜想的解决,"迪利克雷原理"这一数学猜想自提出之日起,历经了三十多年的激烈论争和反复,最终才被确立,这是迪利克雷在研究微分方程位势原理时提出的一个猜想,其具体内容简单地说大体是:极小化迪利克雷积分

$$\iint\left\{\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial u}{\partial y}\right)^2\right\}\mathrm{d}x\mathrm{d}y$$

的函数u,满足位势方程

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$$

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① 海曼·格拉斯曼,《延拓理论》出版于1844年莱比锡.并可参阅其Gesammelte mathematische und physikalische Werke,第1卷,莱比锡,1894年,第二版出版于1898年莱比锡.

② 柏林,1862年.见其著作集第1卷第二部分,莱比锡,1896年.

后来有人在研究三维位势方程(亦称拉普拉斯方程或调和方程)

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}=0$$

时,又提出,由位势方程所描述的相应物理状态总有一个确定的物理解,因而其本身也必然存在一个数学解,但在数学上的这种存在性,长时间的不能被证明,直到1851年,黎曼才在他的博士论文"单复变函数一般理论的基础"中,给出了位势方程边界问题解的存在性证明.由于黎曼在文中运用了他的老师迪利克雷所提出的上述猜想,故他称之为"迪利克雷原理".可是,在其论文发表后的不长时间,这个原理便激起了热烈的讨论,特别是黎曼的这一证明受到了德国著名数学家魏尔斯特拉斯(K. W. Weierstrass,1815—1897)的尖锐批评,他指出:黎曼不加证明就先验地假定一定会存在一个使积分取得到极小值的函数,这在数学上是不允许的,尽管受到了大师的批评,黎曼并没有因此动摇自己对迪利克雷原理的信心,并且一鼓作气又运用此原理作出了一系列重要的发现.1866年,黎曼英年早逝,但关于迪利克雷原理是否成立的争论仍未停止.1870年,魏尔斯特拉斯给出了一个与迪利克雷原理相反的例子,在这个例子中,对给定的边界条件,使迪利克雷积分达到极小值的函数是不存在的,并以此来否定迪利克雷原理.由于迪利克雷原理被当时的数学权威魏尔斯特拉斯所否定,所以数学家们只好另辟蹊径来证明位势方程边界问题解的存在性,比较著名的有三种证法,1870年纽曼用"算术平均值法"给出了一个证明;1890年,许瓦兹用"交替法"又给出了一个证明,同年,庞加莱用"扫散法"也给出了一个证明.这些证明从逻辑上讲无疑都是对的,但就是没有一个能够像以迪利克雷原理为工具那样简单、明快,这又不禁使得数学家们怀念起"迪利克雷原理"来,都对它当年被否定而感到惋惜,并随之产生了复活这一原理的念头,并且也为之做出了一些努力,只可惜都未能成功,数学界为此弥漫着一种悲观的气氛,数学家纽曼就表示:如此优美而又有如此广阔应用前景的迪利克雷原理,已经从我们的视线中"永远消失"掉了!

俗话说"三十年河东,三十年河西",就在迪利克雷原理被否定三十年之后,即1899年,德国领袖数学家希尔伯特对此又发动了一场新的"救亡运动".他彻底冲破了那种把严格性与简单性对立起来的传统观念,批判了魏尔斯特拉斯以严格性全盘否定迪利克雷原理的做法,从迪利克雷原理的简单性、优美性以及应用的有效性出发,积极寻求它的真实性和合理性,最后终于找到了证明迪利克雷原理的途径和方法,他在德国数学联合会上报告了他的这一研究成果,并明确指出:只要对问题中的区域、边界值和允许函数的性质作适当的限制,就完全可以恢复迪利克雷原理的真实性.他还针对数学家们认为迪利克雷原理早已沉没了的观点,意味深长地将他的这一研究工作称为"迪利克雷原理的复活".后来希尔伯特又给出一个更为一般的证明,从而进一步肯定了迪利克雷原理存在的合理性.

及至近代更多源自于物理的数学理论被抽象出来,而对这些数学理论的进一步研究又极大地推动了物理学的进展,如Yang-Mills规范场的大范围整体性质和手征量子反常与纤维丛的拓扑不变量和Chern-Simons示性类及指标定理之间建立起直接的联系,超弦理论中的额外维空间与Calabi-Yan空间之间的对应关系.理论物理学家威腾在发展超弦理论的同时由于对数学的杰出贡献而获得菲尔兹奖,这些都是物理学与数学相互结合所呈现在"数学物理"方面的经典例子.

对此我国数学工作者早有清醒的认识,20世纪80年代李大潜就撰文指出,学数学的追求纯而又纯的境界,即使从纯数学的发展来说,也不见得是一条康庄大道.不重视实际的需要和其他领域的发展,没有广阔的视野,是很难出第一流的基础理论人才的.

基础和应用有着密切的关系,而且相互促进.搞基础理论的人重视应用方面的教育和训练,对基础理论和应用的研究会带来很大的促进.物理学中的规范场和数学上的纤维丛概念有密切的联系.据杨振宁教授自己讲,他在美国请教了很多纤维丛方面的数学家,但他们讲的一套,他听不懂,双方始终谈不到一起去.只有到了复旦大学,听谷超豪教授用物理学家可以接受的语言,把这二者的关系讲得很清楚,杨振宁教授很高兴,并和谷超豪教授合作,在规范场的数学理论方面做出很多成绩,把这方面的理论进一步发展了.为什么能这样呢?谷超豪教授在念大学时,就选修了物理系四大力学的课程.作为一个数学家,他不仅在数学上有很高的造诣,而且在物理学方面也有很好的修养.

从本书的目录我们可以看出它包含了相当全面的数学内容.它们分别是:数学物理学导言、经典力学、流体动力学、可积系统、经典场论、共形与拓扑场论、量子场论、广义相对论、量子引力、弦论与M-理论、凝聚态物质与光学、量子信息与量子计算、量子力学、无序系统、动力系统、平衡态统计力学和非平衡态统计力学、代数技巧、李群和李代数、离散数学、量子群、随机方法、复几何、微分几何、低维几何、非交换几何、代数拓扑、辛几何与拓扑、常微分和偏微分方程、泛函分析和算子代数、量子化方法和路径积分、变分技术.

本书的三位主编在序言中写道:"数学物理把数学和物理学这两大学科的优势集中到一起,它们的关系是共同发展.一方面,它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来;另一方面,物理学家为数学家提供了灵感的源泉."同时,也正如诺贝尔物理学奖获得者荷兰Utrecht大学Gerard't Hooft教授在前言中指出:"物理世界与数学世界之间存在明显的重要区别.物理世界强调事实的'真相',无论'真相'是什么,而数学是纯逻辑和纯推理的世界.在物理

学中,一个理论是否能被接受是由实验来最后决定的.物理学中的方法论也与数学不同."

一个广大读者所关注的例子是天体物理学家霍金是否完美地解决了黑洞火墙悖论?起码现在还没有定论,只能算是给出了第三种可能的解释而已.尽管人们对于黑洞的具体性质还没有全部了解,但是它作为一种致密天体的存在早已没有争议,而黑洞火墙悖论的中心,仍然在于量子力学与广义相对论的矛盾.量子力学把黑洞的视界定义为一个神秘的、拥有巨大能量的火墙,广义相对论则拒绝承认在宇宙中存在这种神奇的火墙,认为黑洞视界只是一种数学上的存在而已.因此,要想真正解决黑洞火墙悖论,人类需要对自然界有更深刻的理解.霍金自己也承认,要想真正理解物质和信息最终从黑洞中逃脱的原理,最终需要人们把引力和自然界的其他作用力合而为一,这是一个困扰了物理学家们将近一个世纪的难题,至今仍然没有得到解决.作为人类现代文明的两块基石,广义相对论通过优美的数学形式描述宇宙,目前人们认为对它已经有足够深刻的理解,而量子力学则通过一种概率化的形式描述微观世界,它的内涵和基本规律仍然不为人知,就连量子力学的创立者尼尔斯·玻尔也说"没有人理解量子力学".黑洞火墙悖论是这两种理论在宇宙深处的交锋,而交锋的结果,目前仍然无法预料.

本书在刚引进中国时曾有过一个12卷精装本.以内容划分是一种创新,这种事出版界常有.

中央文献研究室所编《毛泽东年谱(1949—1976)》(中央文献出版社,2014)皇皇6卷,是读者期待已久的一部大书.不贤者识其小,这里只摘抄一点儿关于图书装订的内容.1965年8月14日,毛泽东就印一批马列经典大字本问题指示周扬:"同意用照相放大胶印的办法.但请注意封面不用硬纸;大书(例如《唯物主义与经验批判主义》《反杜林论》)过去例作一卷或两卷,现应分装4卷或8卷,使每卷重量减轻."印大字本,是因为老同志视力差;封面不用硬纸,就是不要硬精装,因其不方便单手握卷、躺着阅读;较厚的书应该多分几册(其实毛泽东推举的两本书都在500页以下).总体而言,毛泽东对大字本的这些要求,都是以读者为本位,以方便阅读为目的的.有人说:当今出版界在装订方面,流行大开本、大厚本、无线胶订,以傻、大、黑、粗为尚,这种专门为难读者的精神,实在令人费解.

但笔者认为本书绝对算得上是数学物理中的经典之作.而向经典致敬的方式各有不同,最传统、最有效的就是保持原汁原味.原来我们准备连封面都拷贝原版,后与版权代理协商才改成现在的样子.真正美好的东西都一定是增一分则多,减一分则少,原来就刚刚好,我们为什么要破坏它呢?难道我们真的有自信会使其变得更好吗,佛头著粪与狗尾续貂都会让读者吐槽的.

还有一个原因使我们一定要保持原貌,那就是翻译的巨大工作量,我们哈尔滨工业大学出版社地处北方,远离经济与文化中心,实在是没有能力组织宠大的翻译队伍,耗巨资多年打磨这套丛书.我们待将来实力增强后再购买中文版权来完成这一宿愿.在购买版权时我们也表达了购买数字版权的意向,但被婉拒了,因为英文版的数字出版外方已做得很完善了,不像我们刚起步,而且在碎片化之后还面临着版权保护问题,在辞典出版中这是个顽疾.举个例子:

认不认得这个英文单词esquivalience?不认得?那你可以去查一下新版的《新牛津美语词典》(《New Oxford American Dictionary》),里面会告诉你这个词的意思是:"故意逃避自己的官方责任.19世纪开始出现,或许是源自法文esquiver,'躲避,溜走'".

不过如果你拿起家中案头的其他词典,或者将词输入到各种电子词典中,保证你怎么查都查不到这个词,要是你查到了,那可就有事了.

为什么会这样?因为这个词根本就是《新牛津美语词典》编辑部发明的,不存在的词.什么?词典里竟然有虚构的词?编词典的人怎么可以干这种事?

词典里有虚构的词,不只《新牛津美语词典》,基本上每一本词典里都藏有这种凭空创造的词,放这样的词在词典里,倒不是出于编辑的恶作剧坏心,而是有具体用处的.

这是保护著作权的重要机关.辛辛苦苦编出一本厚重的词典,要如何防止别人贪便宜,把你的词典拿去剪剪贴贴,改头换面就变出他们的词典呢?词是共通的,词的意思解释也不会有多大的差别,要怎样证明别人的词典抄袭、盗取你的内容?

要是esquivalience这个词出现在《新牛津美语词典》以外的词典里,就一定牵涉到抄袭、盗取,这个词就是为了找出抄袭、盗取而放在那里埋伏的.

当前全球出版业都不景气,特别是在纸书出版领域.中国出版业尤甚,凉意十足.尽管各路专家给出了不同的原因分析.但只有一位专家给出的答案令业内所信服,那就是优质内容的缺失.说到底出版是一个内容为王的产业,没有好的内容,一切都是无本之源.

有位作家说:平庸是这个时代的危险所在,它无法再吸收传统知识;现代生活杂乱无章,令人湮没无闻.一切都掉在浅水中,没有什么沉入深深的井中;一切都是飞短流长,一切都是流言蜚语.

我们应该敢于承认一个基本事实,这个事实便是——在这个平庸的时代,最坏的都活下来了,最好的死去了,我们这些还能逃生的,发挥不出真正的价值.那么,在这个平庸的时代,我们还能做什么呢?

由衷感谢爱思唯尔(Elsevier)公司于2006年6月出版的这套《Encyclopedia of Mathematical Physics》(《数学物理大百科全书》),这是一部不平凡的全面介绍数学物理知识的百科全书.

本书的三位主编(法国巴黎居里大学 Jean-Pierre Françoise 教授、美国费城德雷塞尔大学 Gregory L. Naber 教授和英国牛津大学 Tsou Sheung Tsun 博士)都是长期从事数学物理方面研究的知名学者.他们邀请了包括诺贝尔物理学奖获得者杨振宁教授和英国牛津大学 Roger Penrose 教授在内的34位著名物理学家和数学家,作为本书的编辑顾问委员会成员,组织来自30个国家的439位在物理学和数学相关研究领域做出杰出贡献的理论物理学家和数学家,撰写了400多篇图文并茂的综述性文章.

《数学物理大百科全书》是经长达4年完成的一部内容全面系统、领域涵盖广泛的百科全书.全书特色鲜明,既体现了学科的基础性、独立性、完整性,又注重学科的前沿性、交叉性、应用性,是当今数学物理研究领域最新和最全的百科全书.

本书内容涉及物理学和数学的几乎各个重要研究领域,遍及从经典力学到量子力学、经典场论到量子场论、共形场论到拓扑场论、流体动力学到动力系统、可积系统到无序系统、粒子物理到天体宇宙学、相对论到量子引力、规范理论到统一理论、平衡态统计到非平衡态统计、凝聚态物质到量子信息、变分技术到代数方法、泛函分析到算子代数、路径积分到随机方法、李群到量子群、微分几何到代数拓扑、低维几何到非交换几何、复几何到辛几何等核心领域和方向.本书还特别注重数学物理的最新研究成果和在各领域的最新应用,并提供了大量必要的和重要的参考文献.

本书相比一般的百科全书有一个明显的亮点是它的综述.它可以告诉你你想知道的某个专题的一切.中国科学院院士赫柏林曾留学于哈尔科夫大学,据他回忆当时的考试是由数学物理教授 A. Ya. Povzner 主持.他出的题目是:"把从你生下来以后所知道的贝塞尔函数的一切都告诉我."据他的学生说:他写了一大摞纸,密密麻麻,然后告诉 Povzner"这是我知道的关于贝塞尔函数知识的提纲.若是需要,我可以展开每一项的具体内容."于是考试通过.

正如 Gerard't Hooft 所指出的那样:

数学物理这个交叉学科是非常难懂的.百科全书中的某些题目纯粹是物理的.高 T_c 超导电性、破坏水波和磁水动力是完全物理的题目,其中的实验数据比任何高深理论都具有决定性.然而,上同调理论、Donaldson-Witten 理论和 AdS/CFT 对应是纯数学的例子.

在编辑中,大量不同作者的短小文章不可避免地被做了适当的变动.在这本百科全书中,理论物理学家和数学家为高等数学物理中的许多重要条目做了简单明了的阐述.所有的文章都包含了供进一步阅读的参考文献.我们盼望这些努力会取得很好的效果.

本书的编者认为:

与狭义的数学和物理学的古老历史相比,数学物理是一门相对较新的独立学科.数学物理国际协会成立于1976年.当然,从古时候起数学与物理学就相互影响.但近几十年来,可能因为我们正身在其中,它们出现了巨大的进展,新的结果和观点以令人目眩的节奏诞生,以至于需要有一本百科全书来搜集整理这些知识.

数学物理把数学和物理学这两个大学科的优势集中到一起,它们的关系是共同发展.一方面,它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来;另一方面,物理学家为数学家们提供了灵感的源泉.两者关系的经典例子是爱因斯坦的相对论,其中微分几何在物理理论的公式化方面起到了实质性的作用,而物理学相继提出的问题推动了微分几何的发展.巧合的是,当我们在为《数学物理大百科全书》写序言时,正值爱因斯坦创造奇迹100周年.

再三考虑到写这部《数学物理大百科全书》是一个艰巨的项目.如果不是坚信这是一项很有意义的、受益于社会的项目,而且我们会得到众多的支持,那么我们绝不会接受这个任务.我们确实获得了许多支持,包括建议、鼓励和有实用性的帮助,这些支持来自编辑顾问委员会成员和我们的作者,还有其他慷慨地抽时间帮我们完善这本百科全书的人.

数学物理是一门较新的学科,它还没有被清晰地刻画,不同的人对它有不同的理解.在我们选择的题目中,一部分遵循了近期数学物理国际大会的纲要,但主要参照编辑顾问委员会和作者的提议.由于时间和空间的限制,以及我们自身的水平所限,更改了某些冗长的题目,但我们尽量收录了我们认为是核心的课题,尽量覆盖更多的最活跃的领域.

近年在中国对本书的原出版商还是有些负面新闻的,起源是在美国一个名为"知识的代价"网站上,已有全球12 196位科学家签名抵制这家世界上最大的出版商.有人用"学术之春"形容这场运动.

吹响号角的是大名鼎鼎的英国数学家威廉·提摩西·高尔斯(William Timothy Gowers).这位来自剑桥大学的菲尔兹奖得主曾发表了一篇博客文章,号召同行行动起来,抵制世界上最大的出版商爱思唯尔集团.

读到这篇博文的泰勒·内伦(Tyler Neylon)——一位目前在硅谷开公司的数学博士当即给高尔斯教授留了言.第二天,他建立了一个网站,命名为"知识的代价".

泰勒事后回忆,自己读到那篇博文,就意识到可以做点什么.在他看来,高尔斯是一位拥有号召力的"超级明星".

迄今为止,数万名科学家在泰勒的网站上签了名.他们发誓,不在爱思唯尔旗下的期刊发论文,不做审稿人,或者不担

任编辑.

尽管如此,我们还是选择了与爱思唯尔的合作,因为一套好的大百科太难得了.

旅法钢琴大师白建宇(Kun-Woo Paik)对钢琴的要求非常苛刻,他在一次与台湾出版人郝明义先生的谈话时说,弹琴弹到现在,职业演奏生涯超过半个世纪,所遇到满意的琴竟不超过5架,如此答案,令见多识广的郝先生也大吃一惊.

在数理方面,近年来国内引进的好的大百科也绝不会超过5部,前苏联五卷本的《数学大百科全书》算一部,日本岩波的《数学百科全书》算一部,总之是屈指可数.

其实这个项目并不是爱思唯尔创始的,据介绍,这个项目开始于 Academic Press,后来由爱思唯尔接手.他们热情的工作人员,把过渡工作做得天衣无缝.并且令人感动的是,相当一部分作者慷慨地把他们的酬劳捐赠给欧洲数学会的发展中国家委员会,我们应该感谢他们为发展中国家所做的一切.

至于我们最关心的问题:谁会去购买这样一套大书,我们充满乐观.大千世界无奇不有,各种购买方式都可能出现.前一阵子,有关霍金打赌输掉关于"上帝粒子"存在性的赌约报道很多.

实验证明霍金输掉了这场赌约,霍金坦承自己输得心服口服并祝愿希格斯获得诺贝尔奖.希格斯透露,在宣布发现新粒子后,霍金曾与他联系并表示支票已寄出.希格斯说,"他不仅是给我一个人钱.我想他还会寄100美元给密歇根大学的戈登·凯恩."

这场赌约的另一位赢家凯恩对来自霍金的美元欣然接受."我坚信希格斯玻色子一定会被找到.发现希格斯玻色子真是太棒了.它证实了长久以来的猜想,进一步加强了粒子物理'标准模型'的事实根据.打赌获胜是锦上添花."凯恩表示要把赢来的钱花在刀刃上,所有的钱都要用于搞研究.

霍金可能已经习惯了以输掉赌约的方式推进科学的普及.

1975年,霍金曾关于天蝎座X—1是否包含黑洞打赌,后来认输,为赢家订阅了1年的《阁楼》杂志.

1991年,霍金又与人赌上了,这次赌的是裸奇点是否存在,霍金再次输了.

第三次打赌发生在1997年,霍金同美国物理学家约翰·普雷斯基尔打赌,认为黑洞部不会摧毁它们吞噬的一切信息,霍金于2004年7月21日当众表示输掉了这场赌约,并送给普雷斯基尔一套板球百科全书.

关于希格斯玻色粒子的赌约则是他的第四场赌约.这30多年来,霍金通过杂志、书籍和一点点美元,让更多的人了解到这些科学最前沿的问题.在100美元的赌约背后,希格斯的远见和霍金的牺牲精神都值得称道.

我们期待下一个赌约会以这样一套百科全书来结束.

著名力学家周培源90岁生日时,北京大学全体师生用"献身科学,教育英才;功在国家,造福将来;寿齐嵩岱,德被春荄;祝嘏欢呼,滴欤盛哉"的贺词赞扬他们的老校长.斗胆借用一下,庆祝这套书在中国的出版,当不为过.

刘培杰

2015年11月1日

于哈工大